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[CN/US]: 4230 Ranwick Court. San Jose. CA 95118 (US). WEHRMAN, Tom [US/US]; CCSR Mol Pharm 3210, 269 W. Campus Drive, Stanford, CA 94305 (US). DRMANAC, Radoie, T. [US/US]: 850 East Greenwich Place, Palo Alto, CA 94303 (US).

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(71) Applicant (for all designated States except US): HYSEQ, INC. [US/US]; 670 Almanor Avenue, Sunnyvalle, CA 94086 (US).

(72) Inventors: and

(75) Inventors/Applicants (for US only): TANG, Y., Tom [US/US]; 4230 Ranwick Court, San Jose, CA 95118 (US). LIU, Chenghua [CN/US]; 1125 Ranchero Way, #14, San Jose, CA 95117 (US). ZHOU, Ping [US/US]; 7595 Newcastle Drive, Cupertino, CA 95014 (US), ASUNDI, Vinod [US/US]; 709 Foster City Boulevard, Foster City, CA 94404 (US). ZHANG, Jie [CN/US]; 4930 Poplar Terrace, Campbell, CA 95008 (US). ZHAO, Qing, A. [CN/US]; 1556 Kooser Road, San Jose, CA 95118 (US). REN, Feiyan [US/US]; 7703 Oak Meadow Court, Cupertino, CA 95014 (US). XUE, Aidong, J. [CN/US]; 1621 S. Mary Avenue, Sunnyvale, CA 94087 (US). YANG, Yonghong (74) Agent: ELRIFI, Ivor, R.; Mintz, Levin, Cohn, Ferris,, Glovsky and Popeo, P.C., One Financial Center, Boston, MA 02111 (US).

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NOVEL NUCLEIC ACIDS AND POLYPEPTIDES

1. TECHNICAL FIELD

The present invention provides novel polynucleotides and proteins encoded by such polynucleotides, along with uses for these polynucleotides and proteins, for example in therapeutic, diagnostic and research methods.

2. BACKGROUND

Technology aimed at the discovery of protein factors (including e.g., cytokines, such as lymphokines, interferons, circulating soluble factors, chemokines, and interleukins) has matured rapidly over the past decade. The now routine hybridization cloning and expression cloning techniques clone novel polynucleotides "directly" in the sense that they rely on information directly related to the discovered protein (i.e., partial DNA/amino acid sequence of the protein in the case of hybridization cloning; activity of the protein in the case of expression cloning). More recent "indirect" cloning techniques such as signal sequence cloning, which isolates DNA sequences based on the presence of a now well-recognized secretory leader sequence motif, as well as various PCR-based or low stringency hybridization-based cloning techniques, have advanced the state of the art by making available large numbers of DNA/amino acid sequences for proteins that are known to have biological activity, for example, by virtue of their secreted nature in the case of leader sequence cloning, by virtue of their cell or tissue source in the case of PCR-based techniques, or by virtue of structural similarity to other genes of known biological activity.

Identified polynucleotide and polypeptide sequences have numerous applications in, for example, diagnostics, forensics, gene mapping; identification of mutations responsible for genetic disorders or other traits, to assess biodiversity, and to produce many other types of data and products dependent on DNA and amino acid sequences.

3. SUMMARY OF THE INVENTION

The compositions of the present invention include novel isolated polypeptides, novel isolated polypucleotides encoding such polypeptides, including recombinant DNA molecules, cloned genes or degenerate variants thereof, especially naturally occurring variants such as allelic variants, antisense polypucleotide molecules, and antibodies that specifically recognize one or more epitopes present on such polypeptides, as well as hybridomas producing such antibodies.

The compositions of the present invention additionally include vectors, including expression vectors, containing the polynucleotides of the invention, cells genetically engineered to contain such polynucleotides and cells genetically engineered to express such polynucleotides.

The present invention relates to a collection or library of at least one novel nucleic acid sequence assembled from expressed sequence tags (ESTs) isolated mainly by sequencing by hybridization (SBH), and in some cases, sequences obtained from one or more public databases. The invention relates also to the proteins encoded by such polynucleotides, along with therapeutic, diagnostic and research utilities for these polynucleotides and proteins. These nucleic acid sequences are designated as SEQ ID NO: 1-444. The polypeptides sequences are designated SEQ ID NO: 445-888. The nucleic acids and polypeptides are provided in the Sequence Listing. In the nucleic acids provided in the Sequence Listing, A is adenosine; C is cytosine; G is guanine; T is thymine; and N is unknown or any of the four bases.

The nucleic acid sequences of the present invention also include, nucleic acid sequences that hybridize to the complement of SEQ ID NO: 1-444 under stringent hybridization conditions; nucleic acid sequences which are allelic variants or species homologues of any of the nucleic acid sequences recited above, or nucleic acid sequences that encode a peptide comprising a specific domain or truncation of the peptides encoded by SEQ ID NO: 1-444. A polynucleotide comprising a nucleotide sequence having at least 90% identity to an identifying sequence of SEQ ID NO: 1-444 or a degenerate variant or fragment thereof. The identifying sequence can be 100 base pairs in length.

The nucleic acid sequences of the present invention also include the sequence information from the nucleic acid sequences of SEQ ID NO: 1-444. The sequence information can be a segment of any one of SEQ ID NO: 1-444 that uniquely identifies or represents the sequence information of SEQ ID NO: 1-444.

A collection as used in this application can be a collection of only one polynucleotide. The collection of sequence information or identifying information of each sequence can be provided on a nucleic acid array. In one embodiment, segments of sequence information are provided on a nucleic acid array to detect the polynucleotide that contains the segment. The array can be designed to detect full-match or mismatch to the polynucleotide that contains the segment. The collection can also be provided in a computer-readable format.

This invention also includes the reverse or direct complement of any of the nucleic acid sequences recited above; cloning or expression vectors containing the nucleic acid sequences; and host cells or organisms transformed with these expression vectors. Nucleic acid sequences (or their reverse or direct complements) according to the invention have numerous applications in a variety of techniques known to those skilled in the art of molecular biology, such as use as hybridization

probes, use as primers for PCR, use in an array, use in computer-readable media, use in sequencing full-length genes, use for chromosome and gene mapping, use in the recombinant production of protein, and use in the generation of anti-sense DNA or RNA, their chemical analogs and the like.

In a preferred embodiment, the nucleic acid sequences of SEQ ID NO: 1-444 or novel segments or parts of the nucleic acids of the invention are used as primers in expression assays that are well known in the art. In a particularly preferred embodiment, the nucleic acid sequences of SEQ ID NO: 1-444 or novel segments or parts of the nucleic acids provided herein are used in diagnostics for identifying expressed genes or, as well known in the art and exemplified by Vollrath et al., Science 258:52-59 (1992), as expressed sequence tags for physical mapping of the human genome.

The isolated polynucleotides of the invention include, but are not limited to, a polynucleotide comprising any one of the nucleotide sequences set forth in SEQ ID NO: 1-444; a polynucleotide comprising any of the full length protein coding sequences of SEQ ID NO: 1-444; and a polynucleotide comprising any of the nucleotide sequences of the mature protein coding sequences of SEQ ID NO: 1-444. The polynucleotides sequences of the mature protein coding sequences of SEQ ID NO: 1-444. The polynucleotides of the present invention also include, but are not limited to, a polynucleotide that hybridizes under stringent hybridization conditions to (a) the complement of any one of the nucleotide sequences set forth in SEQ ID NO: 1-444; (b) a nucleotide sequence encoding any one of the amino acid sequences set forth in the Sequence Listing; (c) a polynucleotide which is an allelic variant of any polynucleotides recited above; (d) a polynucleotide which encodes a species homolog (e.g. orthologs) of any of the proteins recited above; or (e) a polynucleotide that encodes a polypeptide comprising a specific domain or truncation of any of the polypeptides comprising an amino acid sequence set forth in the Sequence Listing.

The isolated polypeptides of the invention include, but are not limited to, a polypeptide comprising any of the amino acid sequences set forth in SEQ ID NO: 445-888; or the corresponding full length or mature protein. Polypeptides of the invention also include polypeptides with biological activity that are encoded by (a) any of the polynucleotides having a nucleotide sequence set forth in SEQ ID NO: 1-444; or (b) polynucleotides that hybridize to the complement of the polynucleotides of (a) under stringent hybridization conditions. Biologically or immunologically active variants of any of the polypeptide sequences in the Sequence Listing, and "substantial equivalents" thereof (e.g., with at least about 65%, 70%, 75%, 80%, 85%, 90%, 95%, 98% or 99% amino acid sequence identity) that preferably retain biological activity are also contemplated. The polypeptides of the invention may be wholly or partially chemically synthesized but are preferably produced by recombinant means using the genetically engineered cells (e.g. host cells) of the invention.

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The invention also provides compositions comprising a polypeptide of the invention.

Polypeptide compositions of the invention may further comprise an acceptable carrier, such as a hydrophilic, e.g., pharmaceutically acceptable, carrier.

The invention also provides host cells transformed or transfected with a polynucleotide of the invention.

The invention also relates to methods for producing a polypeptide of the invention comprising growing a culture of the host cells of the invention in a suitable culture medium under conditions permitting expression of the desired polypeptide, and purifying the polypeptide from the culture or from the host cells. Preferred embodiments include those in which the protein produced by such process is a mature form of the protein.

Polynucleotides according to the invention have numerous applications in a variety of techniques known to those skilled in the art of molecular biology. These techniques include use as hybridization probes, use as oligomers, or primers, for PCR, use for chromosome and gene mapping, use in the recombinant production of protein, and use in generation of anti-sense DNA or RNA, their chemical analogs and the like. For example, when the expression of an mRNA is largely restricted to a particular cell or tissue type, polynucleotides of the invention can be used as hybridization probes to detect the presence of the particular cell or tissue mRNA in a sample using, e.g., in situ hybridization.

In other exemplary embodiments, the polynucleotides are used in diagnostics as expressed sequence tags for identifying expressed genes or, as well known in the art and exemplified by Vollrath et al., Science 258:52-59 (1992), as expressed sequence tags for physical mapping of the human genome.

The polypeptides according to the invention can be used in a variety of conventional procedures and methods that are currently applied to other proteins. For example, a polypeptide of the invention can be used to generate an antibody that specifically binds the polypeptide. Such antibodies, particularly monoclonal antibodies, are useful for detecting or quantitating the polypeptide in tissue. The polypeptides of the invention can also be used as molecular weight markers, and as a food supplement.

Methods are also provided for preventing, treating, or ameliorating a medical condition which comprises the step of administering to a mammalian subject a therapeutically effective amount of a composition comprising a polypeptide of the present invention and a pharmaceutically acceptable carrier.

In particular, the polypeptides and polynucleotides of the invention can be utilized, for example, in methods for the prevention and/or treatment of disorders involving aberrant protein expression or biological activity.

The present invention further relates to methods for detecting the presence of the polynucleotides or polypeptides of the invention in a sample. Such methods can, for example, be utilized as part of prognostic and diagnostic evaluation of disorders as recited herein and for the identification of subjects exhibiting a predisposition to such conditions. The invention provides a method for detecting the polynucleotides of the invention in a sample, comprising contacting the sample with a compound that binds to and forms a complex with the polynucleotide of interest for a period sufficient to form the complex and under conditions sufficient to form a complex and detecting the complex such that if a complex is detected, the polynucleotide of interest is detected. The invention also provides a method for detecting the polypeptides of the invention in a sample comprising contacting the sample with a compound that binds to and forms a complex with the polypeptide under conditions and for a period sufficient to form the complex and detecting the formation of the complex such that if a complex is formed, the polypeptide is detected.

The invention also provides kits comprising polynucleotide probes and/or monoclonal antibodies, and optionally quantitative standards, for carrying out methods of the invention. Furthermore, the invention provides methods for evaluating the efficacy of drugs, and monitoring the progress of patients, involved in clinical trials for the treatment of disorders as recited above.

The invention also provides methods for the identification of compounds that modulate (i.e., increase or decrease) the expression or activity of the polynucleotides and/or polypeptides of the invention. Such methods can be utilized, for example, for the identification of compounds that can ameliorate symptoms of disorders as recited herein. Such methods can include, but are not limited to, assays for identifying compounds and other substances that interact with (e.g., bind to) the polypeptides of the invention. The invention provides a method for identifying a compound that binds to the polypeptides of the invention comprising contacting the compound with a polypeptide of the invention in a cell for a time sufficient to form a polypeptide/compound complex, wherein the complex drives expression of a reporter gene sequence in the cell; and detecting the complex by detecting the reporter gene sequence expression such that if expression of the reporter gene is detected the compound the binds to a polypeptide of the invention is identified.

The methods of the invention also provide methods for treatment which involve the administration of the polynucleotides or polypeptides of the invention to individuals exhibiting symptoms or tendencies. In addition, the invention encompasses methods for treating diseases or disorders as recited herein comprising administering compounds and other substances that modulate the overall activity of the target gene products. Compounds and other substances can

effect such modulation either on the level of target gene/protein expression or target protein activity.

The polypeptides of the present invention and the polynucleotides encoding them are also useful for the same functions known to one of skill in the art as the polypeptides and polynucleotides to which they have homology (set forth in Table 2); for which they have a signature region (as set forth in Table 3); or for which they have homology to a gene family (as set forth in Table 4). If no homology is set forth for a sequence, then the polypeptides and polynucleotides of the present invention are useful for a variety of applications, as described herein, including use in arrays for detection.

4. DETAILED DESCRIPTION OF THE INVENTION

4.1 DEFINITIONS

It must be noted that as used herein and in the appended claims, the singular forms "a", "an" and "the" include plural references unless the context clearly dictates otherwise.

The term "active" refers to those forms of the polypeptide which retain the biologic and/or immunologic activities of any naturally occurring polypeptide. According to the invention, the terms "biologically active" or "biological activity" refer to a protein or peptide having structural, regulatory or biochemical functions of a naturally occurring molecule. Likewise "immunologically active" or "immunological activity" refers to the capability of the natural, recombinant or synthetic polypeptide to induce a specific immune response in appropriate animals or cells and to bind with specific antibodies.

The term "activated cells" as used in this application are those cells which are engaged in extracellular or intracellular membrane trafficking, including the export of secretory or . enzymatic molecules as part of a normal or disease process.

The terms "complementarry" or "complementarity" refer to the natural binding of polynucleotides by base pairing. For example, the sequence 5'-AGT-3' binds to the complementary sequence 3'-TCA-5'. Complementarity between two single-stranded molecules may be "partial" such that only some of the nucleic acids bind or it may be "complete" such that total complementarity exists between the single stranded molecules. The degree of complementarity between the nucleic acid strands has significant effects on the efficiency and strength of the hybridization between the nucleic acid strands.

The term "embryonic stem cells (ES)" refers to a cell that can give rise to many differentiated cell types in an embryo or an adult, including the germ cells. The term "germ line stem cells (GSCs)" refers to stem cells derived from primordial stem cells that provide a steady

and continuous source of germ cells for the production of gametes. The term "primordial germ cells (PGCs)" refers to a small population of cells set aside from other cell lineages particularly from the yolk sac, mesenteries, or gonadal ridges during embryogenesis that have the potential to differentiate into germ cells and other cells. PGCs are the source from which GSCs and ES cells are derived. The PGCs, the GSCs and the ES cells are capable of self-renewal. Thus these cells not only populate the germ line and give rise to a plurality of terminally differentiated cells that comprise the adult specialized organs, but are able to regenerate themselves.

The term "expression modulating fragment," EMF, means a series of nucleotides which modulates the expression of an operably linked ORF or another EMF.

As used herein, a sequence is said to "modulate the expression of an operably linked sequence" when the expression of the sequence is altered by the presence of the EMF. EMFs include, but are not limited to, promoters, and promoter modulating sequences (inducible elements). One class of EMFs are nucleic acid fragments which induce the expression of an operably linked ORF in response to a specific regulatory factor or physiological event.

The terms "nucleotide sequence" or "nucleic acid" or "polynucleotide" or "oligonculeotide" are used interchangeably and refer to a heteropolymer of nucleotides or the sequence of these nucleotides. These phrases also refer to DNA or RNA of genomic or synthetic origin which may be single-stranded or double-stranded and may represent the sense or the antisense strand, to peptide nucleic acid (PNA) or to any DNA-like or RNA-like material. In the sequences herein A is adenine, C is cytosine, T is thymine, G is guanine and N is A, C, G or T (U). It is contemplated that where the polynucleotide is RNA, the T (thymine) in the sequences provided herein is substituted with U (uracil). Generally, nucleic acid segments provided by this invention may be assembled from fragments of the genome and short oligonucleotide linkers, or from a series of oligonucleotides, or from individual nucleotides, to provide a synthetic nucleic acid which is capable of being expressed in a recombinant transcriptional unit comprising regulatory elements derived from a microbial or viral operon, or a eukaryotic gene.

The terms "oligonucleotide fragment" or a "polynucleotide fragment", "portion," or "segment" or "probe" or "primer" are used interchangeably and refer to a sequence of nucleotide residues which are at least about 5 nucleotides, more preferably at least about 7 nucleotides, more preferably at least about 11 nucleotides, more preferably at least about 11 nucleotides and most preferably at least about 17 nucleotides. The fragment is preferably less than about 500 nucleotides, preferably less than about 500 nucleotides, more preferably less than about 50 nucleotides and most preferably less than 30 nucleotides. Preferably the probe is from about 6 nucleotides to about 200 nucleotides, preferably from about 15 to about 50 nucleotides.

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nucleotides and most preferably from about 20 to 25 nucleotides. Preferably the fragments can be used in polymerase chain reaction (PCR), various hybridization procedures or microarray procedures to identify or amplify identical or related parts of mRNA or DNA molecules. A fragment or segment may uniquely identify each polynucleotide sequence of the present invention. Preferably the fragment comprises a sequence substantially similar to any one of SEQ ID NO: 1-444.

Probes may, for example, be used to determine whether specific mRNA molecules are present in a cell or tissue or to isolate similar nucleic acid sequences from chromosomal DNA as described by Walsh et al. (Walsh, P.S. et al., 1992, PCR Methods Appl 1:241-250). They may be labeled by nick translation, Klenow fill-in reaction, PCR, or other methods well known in the art. Probes of the present invention, their preparation and/or labeling are elaborated in Sambrook, J. et al., 1989, Molecular Cloning: A Laboratory Manual, Cold Spring Harbor Laboratory, NY; or Ausubel, F.M. et al., 1989, Current Protocols in Molecular Biology, John Wiley & Sons, New York NY, both of which are incorporated herein by reference in their entirety.

The nucleic acid sequences of the present invention also include the sequence information from the nucleic acid sequences of SEQ ID NO: 1-444. The sequence information can be a segment of any one of SEQ ID NO: 1-444 that uniquely identifies or represents the sequence information of that sequence of SEQ ID NO: 1-444. One such segment can be a twenty-mer nucleic acid sequence because the probability that a twenty-mer is fully matched in the human genome is 1 in 300. In the human genome, there are three billion base pairs in one set of chromosomes. Because 4²⁰ possible twenty-mers exist, there are 300 times more twenty-mers than there are base pairs in a set of human chromosomes. Using the same analysis, the probability for a seventeen-mer to be fully matched in the human genome is approximately 1 in 5. When these segments are used in arrays for expression studies, fifteen-mer segments can be used. The probability that the fifteen-mer is fully matched in the expressed sequences is also approximately one in five because expressed sequences comprise less than approximately 5% of the entire genome sequence.

Similarly, when using sequence information for detecting a single mismatch, a segment can be a twenty-five mer. The probability that the twenty-five mer would appear in a human genome with a single mismatch is calculated by multiplying the probability for a full match (1+4²⁵) times the increased probability for mismatch at each nucleotide position (3 x 25). The probability that an eighteen mer with a single mismatch can be detected in an array for expression studies is approximately one in five. The probability that a twenty-mer with a single mismatch can be detected in a human genome is approximately one in five.

The term "open reading frame," ORF, means a series of nucleotide triplets coding for amino acids without any termination codons and is a sequence translatable into protein.

The terms "operably linked" or "operably associated" refer to functionally related nucleic acid sequences. For example, a promoter is operably associated or operably linked with a coding sequence if the promoter controls the transcription of the coding sequence. While operably linked nucleic acid sequences can be contiguous and in the same reading frame, certain genetic elements e.g. repressor genes are not contiguously linked to the coding sequence but still control transcription/translation of the coding sequence.

The term "pluripotent" refers to the capability of a cell to differentiate into a number of differentiated cell types that are present in an adult organism. A pluripotent cell is restricted in its differentiation capability in comparison to a totipotent cell.

The terms "polypeptide" or "peptide" or "amino acid sequence" refer to an oligopeptide, peptide, polypeptide or protein sequence or fragment thereof and to naturally occurring or synthetic molecules. A polypeptide "fragment," "portion," or "segment" is a stretch of amino acid residues of at least about 5 amino acids, preferably at least about 7 amino acids, more preferably at least about 9 amino acids and most preferably at least about 17 or more amino acids. The peptide preferably is not greater than about 500 amino acids, more preferably less than 200 amino acids more preferably less than 150 amino acids and most preferably less than 100 amino acids. Preferably the peptide is from about 5 to about 200 amino acids. To be active, any polypeptide must have sufficient length to display biological and/or immunological activity.

The term "naturally occurring polypeptide" refers to polypeptides produced by cells that have not been genetically engineered and specifically contemplates various polypeptides arising from post-translational modifications of the polypeptide including, but not limited to, acetylation, carboxylation, glycosylation, phosphorylation, lipidation and acylation.

The term "translated protein coding portion" means a sequence which encodes for the full length protein which may include any leader sequence or any processing sequence.

The term "mature protein coding sequence" means a sequence which encodes a peptide or protein without a signal or leader sequence. The "mature protein portion" means that portion of the protein which does not include a signal or leader sequence. The peptide may have been produced by processing in the cell which removes any leader/signal sequence. The mature protein portion may or may not include an initial methionine residue. The methionine residue may be removed from the protein during processing in the cell. The peptide may be produced synthetically or the protein may have been produced using a polynucleotide only encoding for the mature protein coding sequence.

The term "derivative" refers to polypeptides chemically modified by such techniques as ubiquitination, labeling (e.g., with radionuclides or various enzymes), covalent polymer attachment such as pegylation (derivatization with polyethylene glycol) and insertion or substitution by chemical synthesis of amino acids such as ornithine, which do not normally occur in human proteins.

The term "variant" (or "analog") refers to any polypeptide differing from naturally occurring polypeptides by amino acid insertions, deletions, and substitutions, created using, e.g., recombinant DNA techniques. Guidance in determining which amino acid residues may be replaced, added or deleted without abolishing activities of interest, may be found by comparing the sequence of the particular polypeptide with that of homologous peptides and minimizing the number of amino acid sequence changes made in regions of high homology (conserved regions) or by replacing amino acids with consensus sequence.

Alternatively, recombinant variants encoding these same or similar polypeptides may be synthesized or selected by making use of the "redundancy" in the genetic code. Various codon substitutions, such as the silent changes which produce various restriction sites, may be introduced to optimize cloning into a plasmid or viral vector or expression in a particular prokaryotic or eukaryotic system. Mutations in the polypucleotide sequence may be reflected in the polypeptide or domains of other peptides added to the polypeptide to modify the properties of any part of the polypeptide, to change characteristics such as ligand-binding affinities, interchain affinities, or degradation/turnover rate.

Preferably, amino acid "substitutions" are the result of replacing one amino acid with another amino acid having similar structural and/or chemical properties, i.e., conservative amino acid replacements. "Conservative" amino acid substitutions may be made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity, and/or the amphipathic nature of the residues involved. For example, nonpolar (hydrophobic) amino acids include alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophan, and methionine; polar neutral amino acids include glycine, serine, threonine, cysteine, tyrosine, asparagine, and glutamine; positively charged (basic) amino acids include arginine, lysine, and histidine; and negatively charged (acidic) amino acids include aspartic acid and glutamic acid. "Insertions" or "deletions" are preferably in the range of about 1 to 20 amino acids, more preferably 1 to 10 amino acids. The variation allowed may be experimentally determined by systematically making insertions, deletions, or substitutions of amino acids in a polypeptide molecule using recombinant DNA techniques and assaying the resulting recombinant variants for activity.

Alternatively, where alteration of function is desired, insertions, deletions or non-conservative alterations can be engineered to produce altered polypeptides. Such alterations

can, for example, alter one or more of the biological functions or biochemical characteristics of the polypeptides of the invention. For example, such alterations may change polypeptide characteristics such as ligand-binding affinities, interchain affinities, or degradation/turnover rate. Further, such alterations can be selected so as to generate polypeptides that are better suited for expression, scale up and the like in the host cells chosen for expression. For example, cysteine residues can be deleted or substituted with another amino acid residue in order to eliminate disulfide bridges.

The terms "purified" or "substantially purified" as used herein denotes that the indicated nucleic acid or polypeptide is present in the substantial absence of other biological macromolecules, e.g., polynucleotides, proteins, and the like. In one embodiment, the polynucleotide or polypeptide is purified such that it constitutes at least 95% by weight, more preferably at least 99% by weight, of the indicated biological macromolecules present (but water, buffers, and other small molecules, especially molecules having a molecular weight of less than 1000 daltons, can be present).

The term "isolated" as used herein refers to a nucleic acid or polypeptide separated from at least one other component (e.g., nucleic acid or polypeptide) present with the nucleic acid or polypeptide in its natural source. In one embodiment, the nucleic acid or polypeptide is found in the presence of (if anything) only a solvent, buffer, ion, or other component normally present in a solution of the same. The terms "isolated" and "purified" do not encompass nucleic acids or polypeptides present in their natural source.

The term "recombinant," when used herein to refer to a polypeptide or protein, means that a polypeptide or protein is derived from recombinant (e.g., microbial, insect, or mammalian) expression systems. "Microbial" refers to recombinant polypeptides or proteins made in bacterial or fungal (e.g., yeast) expression systems. As a product, "recombinant microbial" defines a polypeptide or protein essentially free of native endogenous substances and unaccompanied by associated native glycosylation. Polypeptides or proteins expressed in most bacterial cultures, e.g., E. coli, will be free of glycosylation modifications; polypeptides or proteins expressed in yeast will have a glycosylation pattern in general different from those expressed in mammalian cells.

The term "recombinant expression vehicle or vector" refers to a plasmid or phage or virus or vector, for expressing a polypeptide from a DNA (RNA) sequence. An expression vehicle can comprise a transcriptional unit comprising an assembly of (1) a genetic element or elements having a regulatory role in gene expression, for example, promoters or enhancers, (2) a structural or coding sequence which is transcribed into mRNA and translated into protein, and (3) appropriate transcription initiation and termination sequences. Structural units intended for use

in yeast or eukaryotic expression systems preferably include a leader sequence enabling extracellular secretion of translated protein by a host cell. Alternatively, where recombinant protein is expressed without a leader or transport sequence, it may include an amino terminal methionine residue. This residue may or may not be subsequently cleaved from the expressed recombinant protein to provide a final product.

The term "recombinant expression system" means host cells which have stably integrated a recombinant transcriptional unit into chromosomal DNA or carry the recombinant transcriptional unit extrachromosomally. Recombinant expression systems as defined herein will express heterologous polypeptides or proteins upon induction of the regulatory elements linked to the DNA segment or synthetic gene to be expressed. This term also means host cells which have stably integrated a recombinant genetic element or elements having a regulatory role in gene expression, for example, promoters or enhancers. Recombinant expression systems as defined herein will express polypeptides or proteins endogenous to the cell upon induction of the regulatory elements linked to the endogenous DNA segment or gene to be expressed. The cells can be prokaryotic or eukaryotic.

The term "secreted" includes a protein that is transported across or through a membrane, including transport as a result of signal sequences in its amino acid sequence when it is expressed in a suitable host cell. "Secreted" proteins include without limitation proteins secreted wholly (e.g., soluble proteins) or partially (e.g., receptors) from the cell in which they are expressed. "Secreted" proteins also include without limitation proteins that are transported across the membrane of the endoplasmic reticulum. "Secreted" proteins are also intended to include proteins containing non-typical signal sequences (e.g. Interleukin-1 Beta, see Krasney, P.A. and Young, P.R. (1992) Cytokine 4(2): 134-143) and factors released from damaged cells (e.g. Interleukin-1 Receptor Antagonist, see Arend, W.P. et. al. (1998) Annu. Rev. Immunol. 16:27-55)

Where desired, an expression vector may be designed to contain a "signal or leader sequence" which will direct the polypeptide through the membrane of a cell. Such a sequence may be naturally present on the polypeptides of the present invention or provided from heterologous protein sources by recombinant DNA techniques.

The term "stringent" is used to refer to conditions that are commonly understood in the art as stringent. Stringent conditions can include highly stringent conditions (i.e., hybridization to filter-bound DNA in 0.5 M NaHPO₄, 7% sodium dodecyl sulfate (SDS), 1 mM EDTA at 65°C, and washing in 0.1X SSC/0.1% SDS at 68°C), and moderately stringent conditions (i.e., washing in 0.2X SSC/0.1% SDS at 42°C). Other exemplary hybridization conditions are described herein in the examples.

In instances of hybridization of deoxyoligonucleotides, additional exemplary stringent hybridization conditions include washing in 6X SSC/0.05% sodium pyrophosphate at 37°C (for 14-base oligonucleotides), 48°C (for 17-base oligos), 55°C (for 20-base oligonucleotides), and 60°C (for 23-base oligonucleotides).

As used herein, "substantially equivalent" can refer both to nucleotide and amino acid sequences, for example a mutant sequence, that varies from a reference sequence by one or more substitutions, deletions, or additions, the net effect of which does not result in an adverse functional dissimilarity between the reference and subject sequences. Typically, such a substantially equivalent sequence varies from one of those listed herein by no more than about 35% (i.e., the number of individual residue substitutions, additions, and/or deletions in a substantially equivalent sequence, as compared to the corresponding reference sequence, divided by the total number of residues in the substantially equivalent sequence is about 0.35 or less). Such a sequence is said to have 65% sequence identity to the listed sequence. In one embodiment, a substantially equivalent, e.g., mutant, sequence of the invention varies from a listed sequence by no more than 30% (70% sequence identity); in a variation of this embodiment, by no more than 25% (75% sequence identity); and in a further variation of this embodiment, by no more than 20% (80% sequence identity) and in a further variation of this embodiment, by no more than 10% (90% sequence identity) and in a further variation of this embodiment, by no more that 5% (95% sequence identity). Substantially equivalent, e.g., mutant, amino acid sequences according to the invention preferably have at least 80% sequence identity with a listed amino acid sequence, more preferably at least 85% sequence identity, more preferably at least 90% sequence identity, more preferably at least 95% identity, more preferably at least 98% identity, and most preferably at least 99% identity. Substantially equivalent nucleotide sequences of the invention can have lower percent sequence identities, taking into account, for example, the redundancy or degeneracy of the genetic code. Preferably, nucleotide sequence has at least about 65% identity, more preferably at least about 75% identity, more preferably at least about 80% sequence identity, more preferably at least about 85% sequence identity, more preferably at least about 90% sequence identity, and most preferably at least about 95% identity, more preferably at least about 98% sequence identity, and most preferably at least about 99% sequence identity. For the purposes of the present invention, sequences having substantially equivalent biological activity and substantially equivalent expression characteristics are considered substantially equivalent. For the purposes of determining equivalence, truncation of the mature sequence (e.g., via a mutation which creates a spurious stop codon) should be disregarded. Sequence identity may be determined, e.g., using the Jotun Hein method (Hein, J.

(1990) Methods Enzymol. 183:626-645). Identity between sequences can also be determined by other methods known in the art. e.g. by varying hybridization conditions.

The term "totipotent" refers to the capability of a cell to differentiate into all of the cell types of an adult organism.

The term "transformation" means introducing DNA into a suitable host cell so that the DNA is replicable, either as an extrachromosomal element, or by chromosomal integration. The term "transfection" refers to the taking up of an expression vector by a suitable host cell, whether or not any coding sequences are in fact expressed. The term "infection" refers to the introduction of nucleic acids into a suitable host cell by use of a virus or viral vector.

As used herein, an "uptake modulating fragment," UMF, means a series of nucleotides which mediate the uptake of a linked DNA fragment into a cell. UMFs can be readily identified using known UMFs as a target sequence or target motif with the computer-based systems described below. The presence and activity of a UMF can be confirmed by attaching the suspected UMF to a marker sequence. The resulting nucleic acid molecule is then incubated with an appropriate host under appropriate conditions and the uptake of the marker sequence is determined. As described above, a UMF will increase the frequency of uptake of a linked marker sequence.

Each of the above terms is meant to encompass all that is described for each, unless the context dictates otherwise.

4.2 NUCLEIC ACIDS OF THE INVENTION

Nucleotide sequences of the invention are set forth in the Sequence Listing.

The isolated polynucleotides of the invention include a polynucleotide comprising the nucleotide sequences of SEQ ID NO: 1-444; a polynucleotide encoding any one of the peptide sequences of SEQ ID NO: 445-888; and a polynucleotide comprising the nucleotide sequence encoding the mature protein coding sequence of the polypeptides of any one of SEQ ID NO: 445-888. The polynucleotides of the present invention also include, but are not limited to, a polynucleotide that hybridizes under stringent conditions to (a) the complement of any of the nucleotides sequences of SEQ ID NO: 1-444; (b) nucleotide sequences encoding any one of the amino acid sequences set forth in the Sequence Listing as SEQ ID NO: 445-888; (c) a polynucleotide which is an allelic variant of any polynucleotide recited above; (d) a polynucleotide which encodes a species homolog of any of the proteins recited above; or (e) a polynucleotide that encodes a polypeptide comprising a specific domain or truncation of the polypeptides of SEQ ID NO: 445-888. Domains of interest may depend on the nature of the encoded polypeptide; e.g., domains in receptor-like polypeptides include ligand-binding,

extracellular, transmembrane, or cytoplasmic domains, or combinations thereof; domains in immunoglobulin-like proteins include the variable immunoglobulin-like domains; domains in enzyme-like polypeptides include catalytic and substrate binding domains; and domains in ligand polypeptides include receptor-binding domains.

The polynucleotides of the invention include naturally occurring or wholly or partially synthetic DNA, e.g., cDNA and genomic DNA, and RNA, e.g., mRNA. The polynucleotides may include all of the coding region of the cDNA or may represent a portion of the coding region of the cDNA.

The present invention also provides genes corresponding to the cDNA sequences disclosed herein. The corresponding genes can be isolated in accordance with known methods using the sequence information disclosed herein. Such methods include the preparation of probes or primers from the disclosed sequence information for identification and/or amplification of genes in appropriate genomic libraries or other sources of genomic materials. Further 5' and 3' sequence can be obtained using methods known in the art. For example, full length cDNA or genomic DNA that corresponds to any of the polynucleotides of SEQ ID NO: 1-444 can be obtained by screening appropriate cDNA or genomic DNA libraries under suitable hybridization conditions using any of the polynucleotides of SEQ ID NO: 1-444 or a portion thereof as a probe. Alternatively, the polynucleotides of SEQ ID NO: 1-444 may be used as the basis for suitable primer(s) that allow identification and/or amplification of genes in appropriate genomic DNA or cDNA libraries.

The nucleic acid sequences of the invention can be assembled from ESTs and sequences (including cDNA and genomic sequences) obtained from one or more public databases, such as dbEST, gbpri, and UniGene. The EST sequences can provide identifying sequence information, representative fragment or segment information, or novel segment information for the full-length gene.

The polynucleotides of the invention also provide polynucleotides including nucleotide sequences that are substantially equivalent to the polynucleotides recited above. Polynucleotides according to the invention can have, e.g., at least about 65%, at least about 70%, at least about 75%, at least about 80%, 81%, 82%, 83%, 84%, more typically at least about 85%, 86%, 87%, 88%, 89%, more typically at least about 90%, 91%, 92%, 93%, 94%, and even more typically at least about 95%, 96%, 97%, 98%, 99%, sequence identity to a polynucleotide recited above.

Included within the scope of the nucleic acid sequences of the invention are nucleic acid sequence fragments that hybridize under stringent conditions to any of the nucleotide sequences of SEQ ID NO: 1-444, or complements thereof, which fragment is greater than about 5 nucleotides, preferably 7 nucleotides, more preferably greater than 9 nucleotides and most preferably greater than 17 nucleotides. Fragments of, e.g. 15, 17, or 20 nucleotides or more that

are selective for (i.e. specifically hybridize to) any one of the polynucleotides of the invention are contemplated. Probes capable of specifically hybridizing to a polynucleotide can differentiate polynucleotide sequences of the invention from other polynucleotide sequences in the same family of genes or can differentiate human genes from genes of other species, and are preferably based on unique nucleotide sequences.

The sequences falling within the scope of the present invention are not limited to these specific sequences, but also include allelic and species variations thereof. Allelic and species variations can be routinely determined by comparing the sequence provided in SEQ ID NO: 1-444, a representative fragment thereof, or a nucleotide sequence at least 90% identical, preferably 95% identical, to SEQ ID NO: 1-444 with a sequence from another isolate of the same species. Furthermore, to accommodate codon variability, the invention includes nucleic acid molecules coding for the same amino acid sequences as do the specific ORFs disclosed herein. In other words, in the coding region of an ORF, substitution of one codon for another codon that encodes the same amino acid is expressly contemplated.

The nearest neighbor or homology result for the nucleic acids of the present invention, including SEQ ID NO: 1-444, can be obtained by searching a database using an algorithm or a program. Preferably, a BLAST which stands for Basic Local Alignment Search Tool is used to search for local sequence alignments (Altshul, S.F. J Mol. Evol. 36 290-300 (1993) and Altschul S.F. et al. J. Mol. Biol. 21:403-410 (1990)). Alternatively a FASTA version 3 search against Genpept, using Fastsy algorithm.

Species homologs (or orthologs) of the disclosed polynucleotides and proteins are also provided by the present invention. Species homologs may be isolated and identified by making suitable probes or primers from the sequences provided herein and screening a suitable nucleic acid source from the desired species.

The invention also encompasses allelic variants of the disclosed polynucleotides or proteins; that is, naturally-occurring alternative forms of the isolated polynucleotide which also encode proteins which are identical, homologous or related to that encoded by the polynucleotides.

The nucleic acid sequences of the invention are further directed to sequences which encode variants of the described nucleic acids. These amino acid sequence variants may be prepared by methods known in the art by introducing appropriate nucleotide changes into a native or variant polynucleotide. There are two variables in the construction of amino acid sequence variants: the location of the mutation and the nature of the mutation. Nucleic acids encoding the amino acid sequence variants are preferably constructed by mutating the polynucleotide to encode an amino acid sequence that does not occur in nature. These nucleic

acid alterations can be made at sites that differ in the nucleic acids from different species (variable positions) or in highly conserved regions (constant regions). Sites at such locations will typically be modified in series, e.g., by substituting first with conservative choices (e.g., hydrophobic amino acid to a different hydrophobic amino acid) and then with more distant choices (e.g., hydrophobic amino acid to a charged amino acid), and then deletions or insertions may be made at the target site. Amino acid sequence deletions generally range from about 1 to 30 residues, preferably about 1 to 10 residues, and are typically contiguous. Amino acid insertions include amino- and/or carboxyl-terminal fusions ranging in length from one to one hundred or more residues, as well as intrasequence insertions of single or multiple amino acid residues. Intrasequence insertions may range generally from about 1 to 10 amino residues, preferably from 1 to 5 residues. Examples of terminal insertions include the heterologous signal sequences necessary for secretion or for intracellular targeting in different host cells and sequences such as FLAG or poly-histidine sequences useful for purifying the expressed protein.

In a preferred method, polynucleotides encoding the novel amino acid sequences are changed via site-directed mutagenesis. This method uses oligonucleotide sequences to alter a polynucleotide to encode the desired amino acid variant, as well as sufficient adjacent nucleotides on both sides of the changed amino acid to form a stable duplex on either side of the site of being changed. In general, the techniques of site-directed mutagenesis are well known to those of skill in the art and this technique is exemplified by publications such as, Edelman et al., DNA 2:183 (1983). A versatile and efficient method for producing site-specific changes in a polynucleotide sequence was published by Zoller and Smith, Nucleic Acids Res. 10:6487-6500 (1982). PCR may also be used to create amino acid sequence variants of the novel nucleic acids. When small amounts of template DNA are used as starting material, primer(s) that differs slightly in sequence from the corresponding region in the template DNA can generate the desired amino acid variant. PCR amplification results in a population of product DNA fragments that differ from the polynucleotide template encoding the polypeptide at the position specified by the primer. The product DNA fragments replace the corresponding region in the plasmid and this gives a polynucleotide encoding the desired amino acid variant.

A further technique for generating amino acid variants is the cassette mutagenesis technique described in Wells et al., Gene 34:315 (1985); and other mutagenesis techniques well known in the art, such as, for example, the techniques in Sambrook et al., supra, and Current Protocols in Molecular Biology, Ausubel et al. Due to the inherent degeneracy of the genetic code, other DNA sequences which encode substantially the same or a functionally equivalent amino acid sequence may be used in the practice of the invention for the cloning and expression.

of these novel nucleic acids. Such DNA sequences include those which are capable of hybridizing to the appropriate novel nucleic acid sequence under stringent conditions.

Polynucleotides encoding preferred polypeptide truncations of the invention can be used to generate polynucleotides encoding chimeric or fusion proteins comprising one or more domains of the invention and heterologous protein sequences.

The polynucleotides of the invention additionally include the complement of any of the polynucleotides recited above. The polynucleotide can be DNA (genomic, cDNA, amplified, or synthetic) or RNA. Methods and algorithms for obtaining such polynucleotides are well known to those of skill in the art and can include, for example, methods for determining hybridization conditions that can routinely isolate polynucleotides of the desired sequence identities.

In accordance with the invention, polynucleotide sequences comprising the mature protein coding sequences corresponding to any one of SEQ ID NO: 1-444, or functional equivalents thereof, may be used to generate recombinant DNA molecules that direct the expression of that nucleic acid, or a functional equivalent thereof, in appropriate host cells. Also included are the cDNA inserts of any of the clones identified herein.

A polynucleotide according to the invention can be joined to any of a variety of other nucleotide sequences by well-established recombinant DNA techniques (see Sambrook J et al. (1989) Molecular Cloning: A Laboratory Manual, Cold Spring Harbor Laboratory, NY). Useful nucleotide sequences for joining to polynucleotides include an assortment of vectors, e.g., plasmids, cosmids, lambda phage derivatives, phagemids, and the like, that are well known in the art. Accordingly, the invention also provides a vector including a polynucleotide of the invention and a host cell containing the polynucleotide. In general, the vector contains an origin of replication functional in at least one organism, convenient restriction endonuclease sites, and a selectable marker for the host cell. Vectors according to the invention include expression vectors, replication vectors, probe generation vectors, and sequencing vectors. A host cell according to the invention can be a prokaryotic or eukaryotic cell and can be a unicellular organism or part of a multicellular organism.

The present invention further provides recombinant constructs comprising a nucleic acid having any of the nucleotide sequences of SEQ ID NO: 1-444 or a fragment thereof or any other polynucleotides of the invention. In one embodiment, the recombinant constructs of the present invention comprise a vector, such as a plasmid or viral vector, into which a nucleic acid having any of the nucleotide sequences of SEQ ID NO: 1-444 or a fragment thereof is inserted, in a forward or reverse orientation. In the case of a vector comprising one of the ORFs of the present invention, the vector may further comprise regulatory sequences, including for example, a promoter, operably linked to the ORF. Large numbers of suitable vectors and promoters are

known to those of skill in the art and are commercially available for generating the recombinant constructs of the present invention. The following vectors are provided by way of example. Bacterial: pBs, phagescript, PsiX174, pBluescript SK, pBs KS, pNH8a, pNH16a, pNH18a, pNH46a (Stratagene); pTrc99A, pKK223-3, pKK233-3, pDR540, pRIT5 (Pharmacia). Eukaryotic: pWLneo, pSV2cat, pOG44, PXTI, pSG (Stratagene) pSVK3, pBPV, pMSG, pSVL (Pharmacia).

The isolated polynucleotide of the invention may be operably linked to an expression control sequence such as the pMT2 or pED expression vectors disclosed in Kaufman et al., Nucleic Acids Res. 19, 4485-4490 (1991), in order to produce the protein recombinantly. Many suitable expression control sequences are known in the art. General methods of expressing recombinant proteins are also known and are exemplified in R. Kaufman, Methods in Enzymology 185, 537-566 (1990). As defined herein "operably linked" means that the isolated polynucleotide of the invention and an expression control sequence are situated within a vector or cell in such a way that the protein is expressed by a host cell which has been transformed (transfected) with the ligated polynucleotide/expression control sequence.

Promoter regions can be selected from any desired gene using CAT (chloramphenicol transferase) vectors or other vectors with selectable markers. Two appropriate vectors are pKK232-8 and pCM7. Particular named bacterial promoters include lacI, lacZ, T3, T7, gpt. lambda PR, and trc. Eukaryotic promoters include CMV immediate early, HSV thymidine kinase, early and late SV40, LTRs from retrovirus, and mouse metallothionein-I. Selection of the appropriate vector and promoter is well within the level of ordinary skill in the art. Generally, recombinant expression vectors will include origins of replication and selectable markers permitting transformation of the host cell, e.g., the ampicillin resistance gene of E. coli and S. cerevisiae TRP1 gene, and a promoter derived from a highly-expressed gene to direct transcription of a downstream structural sequence. Such promoters can be derived from operons encoding glycolytic enzymes such as 3-phosphoglycerate kinase (PGK), a-factor, acid phosphatase, or heat shock proteins, among others. The heterologous structural sequence is assembled in appropriate phase with translation initiation and termination sequences, and preferably, a leader sequence capable of directing secretion of translated protein into the periplasmic space or extracellular medium. Optionally, the heterologous sequence can encode a fusion protein including an amino terminal identification peptide imparting desired characteristics, e.g., stabilization or simplified purification of expressed recombinant product. Useful expression vectors for bacterial use are constructed by inserting a structural DNA sequence encoding a desired protein together with suitable translation initiation and termination signals in operable reading phase with a functional promoter. The vector will comprise one or

more phenotypic selectable markers and an origin of replication to ensure maintenance of the vector and to, if desirable, provide amplification within the host. Suitable prokaryotic hosts for transformation include *E. coli*, *Bacillus subtilis*, *Salmonella typhimurium* and various species within the genera *Pseudomonas*, *Streptomyces*, and *Staphylococcus*, although others may also be employed as a matter of choice.

As a representative but non-limiting example, useful expression vectors for bacterial use can comprise a selectable marker and bacterial origin of replication derived from commercially available plasmids comprising genetic elements of the well known cloning vector pBR322 (ATCC 37017). Such commercial vectors include, for example, pKK223-3 (Pharmacia Fine Chemicals, Uppsala, Sweden) and GEM 1 (Promega Biotech, Madison, WI, USA). These pBR322 "backbone" sections are combined with an appropriate promoter and the structural sequence to be expressed. Following transformation of a suitable host strain and growth of the host strain to an appropriate cell density, the selected promoter is induced or derepressed by appropriate means (e.g., temperature shift or chemical induction) and cells are cultured for an additional period. Cells are typically harvested by centrifugation, disrupted by physical or chemical means, and the resulting crude extract retained for further purification.

Polynucleotides of the invention can also be used to induce immune responses. For example, as described in Fan et al., Nat. Biotech. 17:870-872 (1999), incorporated herein by reference, nucleic acid sequences encoding a polypeptide may be used to generate antibodies against the encoded polypeptide following topical administration of naked plasmid DNA or following injection, and preferably intramuscular injection of the DNA. The nucleic acid sequences are preferably inserted in a recombinant expression vector and may be in the form of naked DNA.

4.3 ANTISENSE NUCLEIC ACIDS

Another aspect of the invention pertains to isolated antisense nucleic acid molecules that are hybridizable to or complementary to the nucleic acid molecule comprising the nucleotide sequence of SEQ ID NO: 1-444, or fragments, analogs or derivatives thereof. An "antisense" nucleic acid comprises a nucleotide sequence that is complementary to a "sense" nucleic acid encoding a protein, e.g., complementary to the coding strand of a double-stranded cDNA molecule or complementary to an mRNA sequence. In specific aspects, antisense nucleic acid molecules are provided that comprise a sequence complementary to at least about 10, 25, 50, 100, 250 or 500 nucleotides or an entire coding strand, or to only a portion thereof. Nucleic acid molecules encoding fragments, homologs, derivatives and analogs of a protein of any of SEQ ID

NO: 445-888 or antisense nucleic acids complementary to a nucleic acid sequence of SEQ ID NO: 1-444 are additionally provided.

In one embodiment, an antisense nucleic acid molecule is antisense to a "coding region" of the coding strand of a nucleotide sequence of the invention. The term "coding region" refers to the region of the nucleotide sequence comprising codons which are translated into amino acid residues. In another embodiment, the antisense nucleic acid molecule is antisense to a "noncoding region" of the coding strand of a nucleotide sequence of the invention. The term "noncoding region" refers to 5' and 3' sequences which flank the coding region that are not translated into amino acids (i.e., also referred to as 5' and 3' untranslated regions).

Given the coding strand sequences encoding a nucleic acid disclosed herein (e.g., SEQ ID NO: 1-444), antisense nucleic acids of the invention can be designed according to the rules of Watson and Crick or Hoogsteen base pairing. The antisense nucleic acid molecule can be complementary to the entire coding region of an mRNA, but more preferably is an oligonucleotide that is antisense to only a portion of the coding or noncoding region of a mRNA. For example, the antisense oligonucleotide can be complementary to the region surrounding the translation start site of a mRNA. An antisense oligonucleotide can be, for example, about 5, 10, 15, 20, 25, 30, 35, 40, 45 or 50 nucleotides in length. An antisense nucleic acid of the invention can be constructed using chemical synthesis or enzymatic ligation reactions using procedures known in the art. For example, an antisense nucleic acid (e.g., an antisense oligonucleotide) can be chemically synthesized using naturally occurring nucleotides or variously modified nucleotides designed to increase the biological stability of the molecules or to increase the physical stability of the duplex formed between the antisense and sense nucleic acids, e.g., phosphorothioate derivatives and acridine substituted nucleotides can be used.

Examples of modified nucleotides that can be used to generate the antisense nucleic acid include: 5-fluorouracil, 5-bromouracil, 5-chlorouracil, 5-iodouracil, hypoxanthine, xanthine, 4-acetylcytosine, 5-(carboxyhydroxylmethyl) uracil, 5-carboxymethylaminomethyl-2-thiouridine, 5-carboxymethylaminomethyluracil, dihydrouracil, beta-D-galactosylqueosine, inosine, N6-isopentenyladenine, 1-methylguanine, 1-methylinosine, 2,2-dimethylguanine, 2-methyladenine, 2-methylguanine, 5-methylcytosine, N6-adenine, 7-methylguanine, 5-methylcytosine, N6-adenine, 2-methylguanine, 5-methoxyaminomethyl-2-thiouracil, beta-D-mannosylqueosine, 5'-methoxyarboxymethyluracil, 5-methoxyaracil, 2-methylthio-N6-isopentenyladenine, uracil-5-oxyacetic acid (v), wybutoxosine, pseudouracil, queosine, 2-thiocytosine, 5-methyl-2-thiouracil, 2-thiouracil, 5-methyl-2-thiouracil, uracil-5-oxyacetic acid (v), 5-methyl-2-thiouracil, 3-(3-amino-3-N-2-carboxypropyl) uracil, (acp3)w, and 2,6-diaminopurine. Alternatively, the

antisense nucleic acid can be produced biologically using an expression vector into which a nucleic acid has been subcloned in an antisense orientation (i.e., RNA transcribed from the inserted nucleic acid will be of an antisense orientation to a target nucleic acid of interest, described further in the following subsection).

The antisense nucleic acid molecules of the invention are typically administered to a subject or generated in situ such that they hybridize with or bind to cellular mRNA and/or genomic DNA encoding a protein according to the invention to thereby inhibit expression of the protein, e.g., by inhibiting transcription and/or translation. The hybridization can be by conventional nucleotide complementarity to form a stable duplex, or, for example, in the case of an antisense nucleic acid molecule that binds to DNA duplexes, through specific interactions in the major groove of the double helix. An example of a route of administration of antisense nucleic acid molecules of the invention includes direct injection at a tissue site. Alternatively, antisense nucleic acid molecules can be modified to target selected cells and then administered systemically. For example, for systemic administration, antisense molecules can be modified such that they specifically bind to receptors or antigens expressed on a selected cell surface, e.g., by linking the antisense nucleic acid molecules to peptides or antibodies that bind to cell surface receptors or antigens. The antisense nucleic acid molecules can also be delivered to cells using the vectors described herein. To achieve sufficient intracellular concentrations of antisense molecules, vector constructs in which the antisense nucleic acid molecule is placed under the control of a strong pol II or pol III promoter are preferred.

In yet another embodiment, the antisense nucleic acid molecule of the invention is an α -anomeric nucleic acid molecule. An α -anomeric nucleic acid molecule forms specific double-stranded hybrids with complementary RNA in which, contrary to the usual β -units, the strands run parallel to each other (Gaultier *et al.* (1987) *Nucleic Acids Res* 15: 6625-6641). The antisense nucleic acid molecule can also comprise a 2'-o-methylribonucleotide (Inoue *et al.* (1987) *Nucleic Acids Res* 15: 6131-6148) or a chimeric RNA -DNA analogue (Inoue *et al.* (1987) *FEBS Lett* 215: 327-330).

4.4 RIBOZYMES AND PNA MOIETIES

In still another embodiment, an antisense nucleic acid of the invention is a ribozyme. Ribozymes are catalytic RNA molecules with ribonuclease activity that are capable of cleaving a single-stranded nucleic acid, such as an mRNA, to which they have a complementary region. Thus, ribozymes (e.g., hammerhead ribozymes (described in Haselhoff and Gerlach (1988) Nature 334:585-591)) can be used to catalytically cleave a mRNA transcripts to thereby inhibit translation of a mRNA. A ribozyme having specificity for a nucleic acid of the invention can be

designed based upon the nucleotide sequence of a DNA disclosed herein (i.e., SEQ ID NO: 1-444). For example, a derivative of a Tetrahymena L-19 IVS RNA can be constructed in which the nucleotide sequence of the active site is complementary to the nucleotide sequence to be cleaved in an mRNA of SEQ ID NO: 1-444 (see, e.g., Cech et al. U.S. Pat. No. 4,987,071; and Cech et al. U.S. Pat. No. 5,116,742). Alternatively, polynucleotides of the invention can be used to select a catalytic RNA having a specific ribonuclease activity from a pool of RNA molecules. See, e.g., Bartel et al., (1993) Science 261:1411-1418.

Alternatively, gene expression can be inhibited by targeting nucleotide sequences complementary to the regulatory region (e.g., promoter and/or enhancers) to form triple helical structures that prevent transcription of the gene in target cells. See generally, Helene. (1991) Anticancer Drug Des. 6: 569-84; Helene. et al. (1992) Ann. N.Y. Acad. Sci. 660:27-36; and Maher (1992) Bioassays 14: 807-15.

In various embodiments, the nucleic acids of the invention can be modified at the base moiety, sugar moiety or phosphate backbone to improve, e.g., the stability, hybridization, or solubility of the molecule. For example, the deoxyribose phosphate backbone of the nucleic acids can be modified to generate peptide nucleic acids (see Hyrup et al. (1996) Bioorg Med Chem 4: 5-23). As used herein, the terms "peptide nucleic acids" or "PNAs" refer to nucleic acid mimics, e.g., DNA mimics, in which the deoxyribose phosphate backbone is replaced by a pseudopeptide backbone and only the four natural nucleobases are retained. The neutral backbone of PNAs has been shown to allow for specific hybridization to DNA and RNA under conditions of low ionic strength. The synthesis of PNA oligomers can be performed using standard solid phase peptide synthesis protocols as described in Hyrup et al. (1996) above; Perry-O'Keefe et al. (1996) PNAS 93: 14670-675.

PNAs of the invention can be used in therapeutic and diagnostic applications. For example, PNAs can be used as antisense or antigene agents for sequence-specific modulation of gene expression by, e.g., inducing transcription or translation arrest or inhibiting replication. PNAs of the invention can also be used, e.g., in the analysis of single base pair mutations in a gene by, e.g., PNA directed PCR clamping; as artificial restriction enzymes when used in combination with other enzymes, e.g., S1 nucleases (Hyrup B. (1996) above); or as probes or primers for DNA sequence and hybridization (Hyrup et al. (1996), above; Perry-O'Keefe (1996), above).

In another embodiment, PNAs of the invention can be modified, e.g., to enhance their stability or cellular uptake, by attaching lipophilic or other helper groups to PNA, by the formation of PNA-DNA chimeras, or by the use of liposomes or other techniques of drug delivery known in the art. For example, PNA-DNA chimeras can be generated that may

combine the advantageous properties of PNA and DNA. Such chimeras allow DNA recognition enzymes, e.g., RNase H and DNA polymerases, to interact with the DNA portion while the PNA portion would provide high binding affinity and specificity. PNA-DNA chimeras can be linked using linkers of appropriate lengths selected in terms of base stacking, number of bonds between the nucleobases, and orientation (Hyrup (1996) above). The synthesis of PNA-DNA chimeras can be performed as described in Hyrup (1996) above and Finn et al. (1996) Nucl Acids Res 24: 3357-63. For example, a DNA chain can be synthesized on a solid support using standard phosphoramidite coupling chemistry, and modified nucleoside analogs, e.g., 5'-(4-methoxytrityl)amino-5'-deoxy-thymidine phosphoramidite, can be used between the PNA and the 5' end of DNA (Mag et al. (1989) Nucl Acid Res 17: 5973-88). PNA monomers are then coupled in a stepwise manner to produce a chimeric molecule with a 5' PNA segment and a 3' DNA segment (Finn et al. (1996) above). Alternatively, chimeric molecules can be synthesized with a 5' DNA segment and a 3' PNA segment. See, Petersen et al. (1975) Bioorg Med Chem Lett 5: 1119-11124.

In other embodiments, the oligonucleotide may include other appended groups such as peptides (e.g., for targeting host cell receptors in vivo), or agents facilitating transport across the cell membrane (see, e.g., Letsinger et al., 1989, Proc. Natl. Acad. Sci. U.S.A. 86:6553-6556; Lemaitre et al., 1987, Proc. Natl. Acad. Sci. 84:648-652; PCT Publication No. W088/09810) or the blood-brain barrier (see, e.g., PCT Publication No. W089/10134). In addition, oligonucleotides can be modified with hybridization triggered cleavage agents (See, e.g., Krol et al., 1988, BioTechniques 6:958-976) or intercalating agents. (See, e.g., Zon, 1988, Pharm. Res. 5: 539-549). To this end, the oligonucleotide may be conjugated to another molecule, e.g., a peptide, a hybridization triggered cross-linking agent, a transport agent, a hybridization-triggered cleavage agent, etc.

4.5 HOSTS

The present invention further provides host cells genetically engineered to contain the polynucleotides of the invention. For example, such host cells may contain nucleic acids of the invention introduced into the host cell using known transformation, transfection or infection methods. The present invention still further provides host cells genetically engineered to express the polynucleotides of the invention, wherein such polynucleotides are in operative association with a regulatory sequence heterologous to the host cell which drives expression of the polynucleotides in the cell.

Knowledge of nucleic acid sequences allows for modification of cells to permit, or increase, expression of endogenous polypeptide. Cells can be modified (e.g., by homologous

recombination) to provide increased polypeptide expression by replacing, in whole or in part, the naturally occurring promoter with all or part of a heterologous promoter so that the cells express the polypeptide at higher levels. The heterologous promoter is inserted in such a manner that it is operatively linked to the encoding sequences. See, for example, PCT International Publication No. WO94/12650, PCT International Publication No. WO92/20808, and PCT International Publication No. WO91/09955. It is also contemplated that, in addition to heterologous promoter DNA, amplifiable marker DNA (e.g., ada, dhfr, and the multifunctional CAD gene which encodes carbamyl phosphate synthase, aspartate transcarbamylase, and dihydroorotase) and/or intron DNA may be inserted along with the heterologous promoter DNA. If linked to the coding sequence, amplification of the marker DNA by standard selection methods results in co-amplification of the desired protein coding sequences in the cells.

The host cell can be a higher eukaryotic host cell, such as a mammalian cell, a lower eukaryotic host cell, such as a yeast cell, or the host cell can be a prokaryotic cell, such as a bacterial cell. Introduction of the recombinant construct into the host cell can be effected by calcium phosphate transfection, DEAE-dextran mediated transfection, or electroporation (Davis, L. et al., Basic Methods in Molecular Biology (1986)). The host cells containing one of the polynucleotides of the invention, can be used in conventional manners to produce the gene product encoded by the isolated fragment (in the case of an ORF) or can be used to produce a heterologous protein under the control of the EMF.

Any host/vector system can be used to express one or more of the ORFs of the present invention. These include, but are not limited to, eukaryotic hosts such as HeLa cells, Cv-1 cell, COS cells, 293 cells, and Sf9 cells, as well as prokaryotic host such as E. coli and B. subtilis. The most preferred cells are those which do not normally express the particular polypeptide or protein or which expresses the polypeptide or protein at low natural level. Mature proteins can be expressed in mammalian cells, yeast, bacteria, or other cells under the control of appropriate promoters. Cell-free translation systems can also be employed to produce such proteins using RNAs derived from the DNA constructs of the present invention. Appropriate cloning and expression vectors for use with prokaryotic and eukaryotic hosts are described by Sambrook, et al., in Molecular Cloning: A Laboratory Manual, Second Edition, Cold Spring Harbor, New York (1989), the disclosure of which is hereby incomporated by reference.

Various mammalian cell culture systems can also be employed to express recombinant protein. Examples of mammalian expression systems include the COS-7 lines of monkey kidney fibroblasts, described by Gluzman, Cell 23:175 (1981). Other cell lines capable of expressing a compatible vector are, for example, the C127, monkey COS cells, Chinese Hamster Ovary (CHO) cells, human kidney 293 cells, human epidermal A431 cells, human Colo205 cells, 3T3

cells, CV-1 cells, other transformed primate cell lines, normal diploid cells, cell strains derived from *in vitro* culture of primary tissue, primary explants, HeLa cells, mouse L cells, BHK, HL-60, U937, HaK or Jurkat cells. Mammalian expression vectors will comprise an origin of replication, a suitable promoter and also any necessary ribosome binding sites, polyadenylation site, splice donor and acceptor sites, transcriptional termination sequences, and 5' flanking nontranscribed sequences. DNA sequences derived from the SV40 viral genome, for example, SV40 origin, early promoter, enhancer, splice, and polyadenylation sites may be used to provide the required nontranscribed genetic elements. Recombinant polypeptides and proteins produced in bacterial culture are usually isolated by initial extraction from cell pellets, followed by one or more salting-out, aqueous ion exchange or size exclusion chromatography steps. Protein refolding steps can be used, as necessary, in completing configuration of the mature protein. Finally, high performance liquid chromatography (HPLC) can be employed for final purification steps. Microbial cells employed in expression of proteins can be disrupted by any convenient method, including freeze-thaw cycling, sonication, mechanical disruption, or use of cell lysing agents.

Alternatively, it may be possible to produce the protein in lower eukaryotes such as yeast or insects or in prokaryotes such as bacteria. Potentially suitable yeast strains include Saccharomyces cerevisiae, Schizosaccharomyces pombe, Kluyveromyces strains, Candida, or any yeast strain capable of expressing heterologous proteins. Potentially suitable bacterial strains include Escherichia coli, Bacillus subtilis, Salmonella typhimurium, or any bacterial strain capable of expressing heterologous proteins. If the protein is made in yeast or bacteria, it may be necessary to modify the protein produced therein, for example by phosphorylation or glycosylation of the appropriate sites, in order to obtain the functional protein. Such covalent attachments may be accomplished using known chemical or enzymatic methods.

In another embodiment of the present invention, cells and tissues may be engineered to express an endogenous gene comprising the polynucleotides of the invention under the control of inducible regulatory elements, in which case the regulatory sequences of the endogenous gene may be replaced by homologous recombination. As described herein, gene targeting can be used to replace a gene's existing regulatory region with a regulatory sequence isolated from a different gene or a novel regulatory sequence synthesized by genetic engineering methods. Such regulatory sequences may be comprised of promoters, enhancers, scaffold-attachment regions, negative regulatory elements, transcriptional initiation sites, regulatory protein binding sites or combinations of said sequences. Alternatively, sequences which affect the structure or stability of the RNA or protein produced may be replaced, removed, added, or otherwise modified by targeting. These sequence include polyadenylation signals, mRNA stability elements, splice

sites, leader sequences for enhancing or modifying transport or secretion properties of the protein, or other sequences which alter or improve the function or stability of protein or RNA molecules.

The targeting event may be a simple insertion of the regulatory sequence, placing the gene under the control of the new regulatory sequence, e.g., inserting a new promoter or enhancer or both upstream of a gene. Alternatively, the targeting event may be a simple deletion of a regulatory element, such as the deletion of a tissue-specific negative regulatory element. Alternatively, the targeting event may replace an existing element; for example, a tissue-specific enhancer can be replaced by an enhancer that has broader or different cell-type specificity than the naturally occurring elements. Here, the naturally occurring sequences are deleted and new sequences are added. In all cases, the identification of the targeting event may be facilitated by the use of one or more selectable marker genes that are contiguous with the targeting DNA. allowing for the selection of cells in which the exogenous DNA has integrated into the host cell genome. The identification of the targeting event may also be facilitated by the use of one or more marker genes exhibiting the property of negative selection, such that the negatively selectable marker is linked to the exogenous DNA, but configured such that the negatively selectable marker flanks the targeting sequence, and such that a correct homologous recombination event with sequences in the host cell genome does not result in the stable integration of the negatively selectable marker. Markers useful for this purpose include the Herpes Simplex Virus thymidine kinase (TK) gene or the bacterial xanthine-guanine phosphoribosyl-transferase (gpt) gene.

The gene targeting or gene activation techniques which can be used in accordance with this aspect of the invention are more particularly described in U.S. Patent No. 5,272,071 to Chappel; U.S. Patent No. 5,578,461 to Sherwin et al.; International Application No. PCT/US92/09627 (WO93/09222) by Selden et al.; and International Application No. PCT/US90/06436 (WO91/06667) by Skoultchi et al., each of which is incorporated by reference herein in its entirety.

4.6 POLYPEPTIDES OF THE INVENTION

The isolated polypeptides of the invention include, but are not limited to, a polypeptide comprising: the amino acid sequences set forth as any one of SEQ ID NO: 445-888 or an amino acid sequence encoded by any one of the nucleotide sequences SEQ ID NO: 1-444 or the corresponding full length or mature protein. Polypeptides of the invention also include polypeptides preferably with biological or immunological activity that are encoded by: (a) a polynucleotide having any one of the nucleotide sequences set forth in SEQ ID NO: 1-444 or (b)

polynucleotides encoding any one of the amino acid sequences set forth as SEQ ID NO: 445-888 or (c) polynucleotides that hybridize to the complement of the polynucleotides of either (a) or (b) under stringent hybridization conditions. The invention also provides biologically active or immunologically active variants of any of the amino acid sequences set forth as SEQ ID NO: 445-888 or the corresponding full length or mature protein; and "substantial equivalents" thereof (e.g., with at least about 65%, at least about 70%, at least about 75%, at least about 80%, at least about 85%, 86%, 87%, 88%, 89%, at least about 90%, 91%, 92%, 93%, 94%, typically at least about 95%, 96%, 97%, more typically at least about 98%, or most typically at least about 99% amino acid identity) that retain biological activity. Polypeptides encoded by allelic variants may have a similar, increased, or decreased activity compared to polypeptides comprising SEQ ID NO: 445-888.

Fragments of the proteins of the present invention which are capable of exhibiting biological activity are also encompassed by the present invention. Fragments of the protein may be in linear form or they may be cyclized using known methods, for example, as described in H. U. Saragovi, et al., Bio/Technology 10, 773-778 (1992) and in R. S. McDowell, et al., J. Amer. Chem. Soc. 114, 9245-9253 (1992), both of which are incorporated herein by reference. Such fragments may be fused to carrier molecules such as immunoglobulins for many purposes, including increasing the valency of protein binding sites.

The present invention also provides both full-length and mature forms (for example, without a signal sequence or precursor sequence) of the disclosed proteins. The protein coding sequence is identified in the sequence listing by translation of the disclosed nucleotide sequences. The mature form of such protein may be obtained by expression of a full-length polynucleotide in a suitable mammalian cell or other host cell. The sequence of the mature form of the protein is also determinable from the amino acid sequence of the full-length form. Where proteins of the present invention are membrane bound, soluble forms of the proteins are also provided. In such forms, part or all of the regions causing the proteins to be membrane bound are deleted so that the proteins are fully secreted from the cell in which they are expressed.

Protein compositions of the present invention may further comprise an acceptable carrier, such as a hydrophilic, e.g., pharmaceutically acceptable, carrier.

The present invention further provides isolated polypeptides encoded by the nucleic acid fragments of the present invention or by degenerate variants of the nucleic acid fragments of the present invention. By "degenerate variant" is intended nucleotide fragments which differ from a nucleic acid fragment of the present invention (e.g., an ORF) by nucleotide sequence but, due to the degeneracy of the genetic code, encode an identical polypeptide sequence. Preferred nucleic acid fragments of the present invention are the ORFs that encode proteins.

A variety of methodologies known in the art can be utilized to obtain any one of the isolated polypeptides or proteins of the present invention. At the simplest level, the amino acid sequence can be synthesized using commercially available peptide synthesizers. The synthetically-constructed protein sequences, by virtue of sharing primary, secondary or tertiary structural and/or conformational characteristics with proteins may possess biological properties in common therewith, including protein activity. This technique is particularly useful in producing small peptides and fragments of larger polypeptides. Fragments are useful, for example, in generating antibodies against the native polypeptide. Thus, they may be employed as biologically active or immunological substitutes for natural, purified proteins in screening of therapeutic compounds and in immunological processes for the development of antibodies.

The polypeptides and proteins of the present invention can alternatively be purified from cells which have been altered to express the desired polypeptide or protein. As used herein, a cell is said to be altered to express a desired polypeptide or protein when the cell, through genetic manipulation, is made to produce a polypeptide or protein which it normally does not produce or which the cell normally produces at a lower level. One skilled in the art can readily adapt procedures for introducing and expressing either recombinant or synthetic sequences into eukaryotic or prokaryotic cells in order to generate a cell which produces one of the polypeptides or proteins of the present invention.

The invention also relates to methods for producing a polypeptide comprising growing a culture of host cells of the invention in a suitable culture medium, and purifying the protein from the cells or the culture in which the cells are grown. For example, the methods of the invention include a process for producing a polypeptide in which a host cell containing a suitable expression vector that includes a polynucleotide of the invention is cultured under conditions that allow expression of the encoded polypeptide. The polypeptide can be recovered from the culture, conveniently from the culture medium, or from a lysate prepared from the host cells and further purified. Preferred embodiments include those in which the protein produced by such process is a full length or mature form of the protein.

In an alternative method, the polypeptide or protein is purified from bacterial cells which naturally produce the polypeptide or protein. One skilled in the art can readily follow known methods for isolating polypeptides and proteins in order to obtain one of the isolated polypeptides or proteins of the present invention. These include, but are not limited to, immunochromatography, HPLC, size-exclusion chromatography, ion-exchange chromatography, and immuno-affinity chromatography. See, e.g., Scopes, Protein Purification: Principles and Practice, Springer-Verlag (1994); Sambrook, et al., in Molecular Cloning: A Laboratory Manual; Ausubel et al., Current Protocols in Molecular Biology. Polypeptide fragments that

retain biological/immunological activity include fragments comprising greater than about 100 amino acids, or greater than about 200 amino acids, and fragments that encode specific protein domains.

The purified polypeptides can be used in in vitro binding assays which are well known in the art to identify molecules which bind to the polypeptides. These molecules include but are not limited to, for e.g., small molecules, molecules from combinatorial libraries, antibodies or other proteins. The molecules identified in the binding assay are then tested for antagonist or agonist activity in in vivo tissue culture or animal models that are well known in the art. In brief, the molecules are titrated into a plurality of cell cultures or animals and then tested for either cell/animal death or prolonged survival of the animal/cells.

In addition, the peptides of the invention or molecules capable of binding to the peptides may be complexed with toxins, e.g., ricin or cholera, or with other compounds that are toxic to cells. The toxin-binding molecule complex is then targeted to a tumor or other cell by the specificity of the binding molecule for SEO ID NO: 445-888.

The protein of the invention may also be expressed as a product of transgenic animals, e.g., as a component of the milk of transgenic cows, goats, pigs, or sheep which are characterized by somatic or germ cells containing a nucleotide sequence encoding the protein.

The proteins provided herein also include proteins characterized by amino acid sequences similar to those of purified proteins but into which modification are naturally provided or deliberately engineered. For example, modifications, in the peptide or DNA sequence, can be made by those skilled in the art using known techniques. Modifications of interest in the protein sequences may include the alteration, substitution, replacement, insertion or deletion of a selected amino acid residue in the coding sequence. For example, one or more of the cysteine residues may be deleted or replaced with another amino acid to alter the conformation of the molecule. Techniques for such alteration, substitution, replacement, insertion or deletion are well known to those skilled in the art (see, e.g., U.S. Pat. No. 4,518,584). Preferably, such alteration, substitution, replacement, insertion or deletion retains the desired activity of the protein. Regions of the protein that are important for the protein function can be determined by various methods known in the art including the alanine-scanning method which involved systematic substitution of single or strings of amino acids with alanine, followed by testing the resulting alanine-containing variant for biological activity. This type of analysis determines the importance of the substituted amino acid(s) in biological activity. Regions of the protein that are important for protein function may be determined by the eMATRIX program.

Other fragments and derivatives of the sequences of proteins which would be expected to retain protein activity in whole or in part and are useful for screening or other immunological

methodologies may also be easily made by those skilled in the art given the disclosures herein.

Such modifications are encompassed by the present invention.

The protein may also be produced by operably linking the isolated polynucleotide of the invention to suitable control sequences in one or more insect expression vectors, and employing an insect expression system. Materials and methods for baculovirus/insect cell expression systems are commercially available in kit form from, e.g., Invitrogen, San Diego, Calif., U.S.A. (the MaxBatTM kit), and such methods are well known in the art, as described in Summers and Smith, Texas Agricultural Experiment Station Bulletin No. 1555 (1987), incorporated herein by reference. As used herein, an insect cell capable of expressing a polynucleotide of the present invention is "transformed."

The protein of the invention may be prepared by culturing transformed host cells under culture conditions suitable to express the recombinant protein. The resulting expressed protein may then be purified from such culture (i.e., from culture medium or cell extracts) using known purification processes, such as gel filtration and ion exchange chromatography. The purification of the protein may also include an affinity column containing agents which will bind to the protein; one or more column steps over such affinity resins as concanavalin A-agarose, heparin-toyopearlTM or Cibacrom blue 3GA SepharoseTM; one or more steps involving hydrophobic interaction chromatography using such resins as phenyl ether, butyl ether, or propyl ether; or immunoaffinity chromatography.

Alternatively, the protein of the invention may also be expressed in a form which will facilitate purification. For example, it may be expressed as a fusion protein, such as those of maltose binding protein (MBP), glutathione-S-transferase (GST) or thioredoxin (TRX), or as a His tag. Kits for expression and purification of such fusion proteins are commercially available from New England BioLab (Beverly, Mass.), Pharmacia (Piscataway, N.J.) and Invitrogen, respectively. The protein can also be tagged with an epitope and subsequently purified by using a specific antibody directed to such epitope. One such epitope ("FLAG®") is commercially available from Kodak (New Haven, Conn.).

Finally, one or more reverse-phase high performance liquid chromatography (RP-HPLC) steps employing hydrophobic RP-HPLC media, e.g., silica gel having pendant methyl or other aliphatic groups, can be employed to further purify the protein. Some or all of the foregoing purification steps, in various combinations, can also be employed to provide a substantially homogeneous isolated recombinant protein. The protein thus purified is substantially free of other mammalian proteins and is defined in accordance with the present invention as an "isolated protein."

The polypeptides of the invention include analogs (variants). This embraces fragments, as well as peptides in which one or more amino acids has been deleted, inserted, or substituted. Also, analogs of the polypeptides of the invention embrace fusions of the polypeptides or modifications of the polypeptides of the invention, wherein the polypeptide or analog is fused to another moiety or moieties, e.g., targeting moiety or another therapeutic agent. Such analogs may exhibit improved properties such as activity and/or stability. Examples of moieties which may be fused to the polypeptide or an analog include, for example, targeting moieties which provide for the delivery of polypeptide to pancreatic cells, e.g., antibodies to pancreatic cells, antibodies to immune cells such as T-cells, monocytes, dendritic cells, granulocytes, etc., as well as receptor and ligands expressed on pancreatic or immune cells. Other moieties which may be fused to the polypeptide include therapeutic agents which are used for treatment, for example, immunosuppressive drugs such as cyclosporin, SK506, azathioprine, CD3 antibodies and steroids. Also, polypeptides may be fused to immune modulators, and other cytokines such as alpha or beta interferon.

4.6.1 DETERMINING POLYPEPTIDE AND POLYNUCLEOTIDE IDENTITY AND SIMILARITY

Preferred identity and/or similarity are designed to give the largest match between the sequences tested. Methods to determine identity and similarity are codified in computer programs including, but are not limited to, the GCG program package, including GAP (Devereux, J., et al., Nucleic Acids Research 12(1):387 (1984); Genetics Computer Group, University of Wisconsin, Madison, WI), BLASTP, BLASTN, BLASTX, FASTA (Altschul, S.F. et al., J. Molec. Biol. 215:403-410 (1990), PSI-BLAST (Altschul S.F. et al., Nucleic Acids Res. vol. 25, pp. 3389-3402, herein incorporated by reference), eMatrix software (Wu et al., J. Comp. Biol., Vol. 6, pp. 219-235 (1999), herein incorporated by reference), eMotif software (Nevill-Manning et al, ISMB-97, Vol. 4, pp. 202-209, herein incorporated by reference), pFam software (Sonnhammer et al., Nucleic Acids Res., Vol. 26(1), pp. 320-322 (1998), herein incorporated by reference), the GeneAtlas software (Molecular Simulations Inc. (MSI), San Diego, CA) (Sanchez and Sali (1998) Proc. Natl. Acad. Sci., 95, 13597-13602; Kitson DH et al. (2000) "Remote homology detection using structural modeling - an evaluation" Submitted; Fischer and Eisenberg (1996) Protein Sci. 5, 947-955), Neural Network SignalP V1.1 program (from Center for Biological Sequence Analysis, The Technical University of Denmark), and the Kyte-Doolittle hydrophobocity prediction algorithm (J. Mol Biol, 157, pp. 105-31 (1982), incorporated herein by reference). The BLAST programs are publicly available from the National Center for Biotechnology Information (NCBI) and other sources (BLAST Manual,

Altschul, S., et al. NCB NLM NIH Bethesda, MD 20894; Altschul, S., et al., J. Mol. Biol. 215:403-410 (1990).

4.7 CHIMERIC AND FUSION PROTEINS

The invention also provides chimeric or fusion proteins. As used herein, a "chimeric protein" or "fusion protein" comprises a polypeptide of the invention operatively linked to another polypeptide. Within a fusion protein the polypeptide according to the invention can correspond to all or a portion of a protein according to the invention. In one embodiment, a fusion protein comprises at least one biologically active portion of a protein according to the invention. In another embodiment, a fusion protein comprises at least two biologically active portions of a protein according to the invention. Within the fusion protein, the term "operatively linked" is intended to indicate that the polypeptide according to the invention and the other polypeptide are fused in-frame to each other. The polypeptide can be fused to the N-terminus or C-terminus.

For example, in one embodiment a fusion protein comprises a polypeptide according to the invention operably linked to the extracellular domain of a second protein.

In another embodiment, the fusion protein is a GST-fusion protein in which the polypeptide sequences of the invention are fused to the C-terminus of the GST (i.e., glutathione S-transferase) sequences.

In another embodiment, the fusion protein is an immunoglobulin fusion protein in which the polypeptide sequences according to the invention comprise one or more domains fused to sequences derived from a member of the immunoglobulin protein family. The immunoglobulin fusion proteins of the invention can be incorporated into pharmaceutical compositions and administered to a subject to inhibit an interaction between a ligand and a protein of the invention on the surface of a cell, to thereby suppress signal transduction in vivo. The immunoglobulin fusion proteins can be used to affect the bioavailability of a cognate ligand. Inhibition of the ligand/protein interaction may be useful therapeutically for both the treatment of proliferative and differentiative disorders, e.g., cancer as well as modulating (e.g., promoting or inhibiting) cell survival. Moreover, the immunoglobulin fusion proteins of the invention can be used as immunogens to produce antibodies in a subject, to purify ligands, and in screening assays to identify molecules that inhibit the interaction of a polypeptide of the invention with a ligand.

A chimeric or fusion protein of the invention can be produced by standard recombinant DNA techniques. For example, DNA fragments coding for the different polypeptide sequences are ligated together in-frame in accordance with conventional techniques, e.g., by employing blunt-ended or stagger-ended termini for ligation, restriction enzyme digestion to provide for appropriate termini, filling-in of cohesive ends as appropriate, alkaline phosphatase treatment to

avoid undesirable joining, and enzymatic ligation. In another embodiment, the fusion gene can be synthesized by conventional techniques including automated DNA synthesizers.

Alternatively, PCR amplification of gene fragments can be carried out using anchor primers that give rise to complementary overhangs between two consecutive gene fragments that can subsequently be annealed and reamplified to generate a chimeric gene sequence (see, for example, Ausubel et al. (eds.) CURRENT PROTOCOLS IN MOLECULAR BIOLOGY, John Wiley & Sons, 1992). Moreover, many expression vectors are commercially available that already encode a fusion moiety (e.g., a GST polypeptide). A nucleic acid encoding a polypeptide of the invention can be cloned into such an expression vector such that the fusion moiety is linked in-frame to the protein of the invention.

4.8 GENE THERAPY

Mutations in the polynucleotides of the invention may result in loss of normal function of the encoded protein. The invention thus provides gene therapy to restore normal activity of the polypeptides of the invention; or to treat disease states involving polypeptides of the invention. Delivery of a functional gene encoding polypeptides of the invention to appropriate cells is effected ex vivo, in situ, or in vivo by use of vectors, and more particularly viral vectors (e.g., adenovirus, adeno-associated virus, or a retrovirus), or ex vivo by use of physical DNA transfer methods (e.g., liposomes or chemical treatments). See, for example, Anderson, Nature, supplement to vol. 392, no. 6679, pp.25-20 (1998). For additional reviews of gene therapy technology see Friedmann, Science, 244: 1275-1281 (1989); Verma, Scientific American: 68-84 (1990); and Miller, Nature, 357: 455-460 (1992). Introduction of any one of the nucleotides of the present invention or a gene encoding the polypeptides of the present invention can also be accomplished with extrachromosomal substrates (transient expression) or artificial chromosomes (stable expression). Cells may also be cultured ex vivo in the presence of proteins of the present invention in order to proliferate or to produce a desired effect on or activity in such cells. Treated cells can then be introduced in vivo for therapeutic purposes. Alternatively, it is contemplated that in other human disease states, preventing the expression of or inhibiting the activity of polypeptides of the invention will be useful in treating the disease states. It is contemplated that antisense therapy or gene therapy could be applied to negatively regulate the expression of polypeptides of the invention.

Other methods inhibiting expression of a protein include the introduction of antisense molecules to the nucleic acids of the present invention, their complements, or their translated RNA sequences, by methods known in the art. Further, the polypeptides of the present invention can be

inhibited by using targeted deletion methods, or the insertion of a negative regulatory element such as a silencer, which is tissue specific.

The present invention still further provides cells genetically engineered in vivo to express the polynucleotides of the invention, wherein such polynucleotides are in operative association with a regulatory sequence heterologous to the host cell which drives expression of the polynucleotides in the cell. These methods can be used to increase or decrease the expression of the polynucleotides of the present invention.

Knowledge of DNA sequences provided by the invention allows for modification of cells to permit, increase, or decrease, expression of endogenous polypeptide. Cells can be modified (e.g., by homologous recombination) to provide increased polypeptide expression by replacing, in whole or in part, the naturally occurring promoter with all or part of a heterologous promoter so that the cells express the protein at higher levels. The heterologous promoter is inserted in such a manner that it is operatively linked to the desired protein encoding sequences. See, for example, PCT International Publication No. WO 94/12650, PCT International Publication No. WO 92/20808, and PCT International Publication No. WO 91/09955. It is also contemplated that, in addition to heterologous promoter DNA, amplifiable marker DNA (e.g., ada, dhfr, and the multifunctional CAD gene which encodes carbamyl phosphate synthase, aspartate transcarbamylase, and dihydroorotase) and/or intron DNA may be inserted along with the heterologous promoter DNA. If linked to the desired protein coding sequence, amplification of the marker DNA by standard selection methods results in co-amplification of the desired protein coding sequences in the cells.

In another embodiment of the present invention, cells and tissues may be engineered to express an endogenous gene comprising the polynucleotides of the invention under the control of inducible regulatory elements, in which case the regulatory sequences of the endogenous gene may be replaced by homologous recombination. As described herein, gene targeting can be used to replace a gene's existing regulatory region with a regulatory sequence isolated from a different gene or a novel regulatory sequence synthesized by genetic engineering methods. Such regulatory sequences may be comprised of promoters, enhancers, scaffold-attachment regions, negative regulatory elements, transcriptional initiation sites, regulatory protein binding sites or combinations of said sequences. Alternatively, sequences which affect the structure or stability of the RNA or protein produced may be replaced, removed, added, or otherwise modified by targeting. These sequences include polyadenylation signals, mRNA stability elements, splice sites, leader sequences for enhancing or modifying transport or secretion properties of the protein, or other sequences which alter or improve the function or stability of protein or RNA molecules.

The targeting event may be a simple insertion of the regulatory sequence, placing the gene under the control of the new regulatory sequence, e.g., inserting a new promoter or enhancer or both

upstream of a gene. Alternatively, the targeting event may be a simple deletion of a regulatory element, such as the deletion of a tissue-specific negative regulatory element. Alternatively, the targeting event may replace an existing element; for example, a tissue-specific enhancer can be replaced by an enhancer that has broader or different cell-type specificity than the naturally occurring elements. Here, the naturally occurring sequences are deleted and new sequences are added. In all cases, the identification of the targeting event may be facilitated by the use of one or more selectable marker genes that are contiguous with the targeting DNA, allowing for the selection of cells in which the exogenous DNA has integrated into the cell genome. The identification of the targeting event may also be facilitated by the use of one or more marker genes exhibiting the property of negative selection, such that the negatively selectable marker is linked to the exogenous DNA, but configured such that the negatively selectable marker flanks the targeting sequence, and such that a correct homologous recombination event with sequences in the host cell genome does not result in the stable integration of the negatively selectable marker. Markers useful for this purpose include the Herpes Simplex Virus thymidine kinase (TK) gene or the bacterial xanthine-guanine phosphoribosyl-transferase (gpt) gene.

The gene targeting or gene activation techniques which can be used in accordance with this aspect of the invention are more particularly described in U.S. Patent No. 5,272,071 to Chappel; U.S. Patent No. 5,578,461 to Sherwin et al.; International Application No. PCT/US92/09627 (WO93/09222) by Selden et al.; and International Application No. PCT/US90/06436 (WO91/06667) by Skoultchi et al., each of which is incorporated by reference herein in its entirety.

4.9 TRANSGENIC ANIMALS

In preferred methods to determine biological functions of the polypeptides of the invention in vivo, one or more genes provided by the invention are either over expressed or inactivated in the germ line of animals using homologous recombination [Capecchi, Science 244:1288-1292 (1989)]. Animals in which the gene is over expressed, under the regulatory control of exogenous or endogenous promoter elements, are known as transgenic animals. Animals in which an endogenous gene has been inactivated by homologous recombination are referred to as "knockout" animals. Knockout animals, preferably non-human mammals, can be prepared as described in U.S. Patent No. 5,557,032, incorporated herein by reference. Transgenic animals are useful to determine the roles polypeptides of the invention play in biological processes, and preferably in disease states. Transgenic animals are useful as model systems to identify compounds that modulate lipid metabolism. Transgenic animals, preferably non-human mammals, are produced using methods as described in U.S. Patent No 5,489,743 and PCT Publication No. WO94/28122, incorporated herein by reference.

Transgenic animals can be prepared wherein all or part of a promoter of the polynucleotides of the invention is either activated or inactivated to alter the level of expression of the polypeptides of the invention. Inactivation can be carried out using homologous recombination methods described above. Activation can be achieved by supplementing or even replacing the homologous promoter to provide for increased protein expression. The homologous promoter can be supplemented by insertion of one or more heterologous enhancer elements known to confer promoter activation in a particular tissue.

The polynucleotides of the present invention also make possible the development, through, e.g., homologous recombination or knock out strategies, of animals that fail to express polypeptides of the invention or that express a variant polypeptide. Such animals are useful as models for studying the *in vivo* activities of polypeptide as well as for studying modulators of the polypeptides of the invention.

In preferred methods to determine biological functions of the polypeptides of the invention in vivo, one or more genes provided by the invention are either over expressed or inactivated in the germ line of animals using homologous recombination [Capecchi, Science 244:1288-1292 (1989)]. Animals in which the gene is over expressed, under the regulatory control of exogenous or endogenous promoter elements, are known as transgenic animals. Animals in which an endogenous gene has been inactivated by homologous recombination are referred to as "knockout" animals. Knockout animals, preferably non-human mammals, can be prepared as described in U.S. Patent No. 5,557,032, incorporated herein by reference. Transgenic animals are useful to determine the roles polypeptides of the invention play in biological processes, and preferably in disease states. Transgenic animals are useful as model systems to identify compounds that modulate lipid metabolism. Transgenic animals, preferably non-human mammals, are produced using methods as described in U.S. Patent No 5,489,743 and PCT Publication No. WO94/28122, incorporated herein by reference.

Transgenic animals can be prepared wherein all or part of the polynucleotides of the invention promoter is either activated or inactivated to alter the level of expression of the polypeptides of the invention. Inactivation can be carried out using homologous recombination methods described above. Activation can be achieved by supplementing or even replacing the homologous promoter to provide for increased protein expression. The homologous promoter can be supplemented by insertion of one or more heterologous enhancer elements known to confer promoter activation in a particular tissue.

4.10 USES AND BIOLOGICAL ACTIVITY

The polynucleotides and proteins of the present invention are expected to exhibit one or more of the uses or biological activities (including those associated with assays cited herein) identified herein. Uses or activities described for proteins of the present invention may be provided by administration or use of such proteins or of polynucleotides encoding such proteins (such as, for example, in gene therapies or vectors suitable for introduction of DNA). The mechanism underlying the particular condition or pathology will dictate whether the polypeptides of the invention, the polynucleotides of the invention or modulators (activators or inhibitors) thereof would be beneficial to the subject in need of treatment. Thus, "therapeutic compositions of the invention" include compositions comprising isolated polynucleotides (including recombinant DNA molecules, cloned genes and degenerate variants thereof) or polypeptides of the invention (including full length protein, mature protein and truncations or domains thereof), or compounds and other substances that modulate the overall activity of the target gene products, either at the level of target gene/protein expression or target protein activity. Such modulators include polypeptides, analogs, (variants), including fragments and fusion proteins, antibodies and other binding proteins; chemical compounds that directly or indirectly activate or inhibit the polypeptides of the invention (identified, e.g., via drug screening assays as described herein); antisense polynucleotides and polynucleotides suitable for triple helix formation; and in particular antibodies or other binding partners that specifically recognize one or more epitopes of the polypeptides of the invention.

The polypeptides of the present invention may likewise be involved in cellular activation or in one of the other physiological pathways described herein.

4.10.1 RESEARCH USES AND UTILITIES

The polynucleotides provided by the present invention can be used by the research community for various purposes. The polynucleotides can be used to express recombinant protein for analysis, characterization or therapeutic use; as markers for tissues in which the corresponding protein is preferentially expressed (either constitutively or at a particular stage of tissue differentiation or development or in disease states); as molecular weight markers on gels; as chromosome markers or tags (when labeled) to identify chromosomes or to map related gene positions; to compare with endogenous DNA sequences in patients to identify potential genetic disorders; as probes to hybridize and thus discover novel, related DNA sequences; as a source of information to derive PCR primers for genetic fingerprinting; as a probe to "subtract-out" known sequences in the process of discovering other novel polynucleotides; for selecting and making oligomers for attachment to a "gene chip" or other support, including for examination of expression patterns; to raise anti-protein antibodies using DNA immunization techniques; and as

an antigen to raise anti-DNA antibodies or elicit another immune response. Where the polynucleotide encodes a protein which binds or potentially binds to another protein (such as, for example, in a receptor-ligand interaction), the polynucleotide can also be used in interaction trap assays (such as, for example, that described in Gyuris et al., Cell 75:791-803 (1993)) to identify polynucleotides encoding the other protein with which binding occurs or to identify inhibitors of the binding interaction.

The polypeptides provided by the present invention can similarly be used in assays to determine biological activity, including in a panel of multiple proteins for high-throughput screening; to raise antibodies or to elicit another immune response; as a reagent (including the labeled reagent) in assays designed to quantitatively determine levels of the protein (or its receptor) in biological fluids; as markers for tissues in which the corresponding polypeptide is preferentially expressed (either constitutively or at a particular stage of tissue differentiation or development or in a disease state); and, of course, to isolate correlative receptors or ligands. Proteins involved in these binding interactions can also be used to screen for peptide or small molecule inhibitors or agonists of the binding interaction.

Any or all of these research utilities are capable of being developed into reagent grade or kit format for commercialization as research products.

Methods for performing the uses listed above are well known to those skilled in the art. References disclosing such methods include without limitation "Molecular Cloning: A Laboratory Manual", 2d ed., Cold Spring Harbor Laboratory Press, Sambrook, J., E. F. Fritsch and T. Maniatis eds., 1989, and "Methods in Enzymology: Guide to Molecular Cloning Techniques", Academic Press, Berger, S. L. and A. R. Kimmel eds., 1987.

4.10.2 NUTRITIONAL USES

Polynucleotides and polypeptides of the present invention can also be used as nutritional sources or supplements. Such uses include without limitation use as a protein or amino acid supplement, use as a carbon source, use as a nitrogen source and use as a source of carbohydrate. In such cases the polypeptide or polynucleotide of the invention can be added to the feed of a particular organism or can be administered as a separate solid or liquid preparation, such as in the form of powder, pills, solutions, suspensions or capsules. In the case of microorganisms, the polypeptide or polynucleotide of the invention can be added to the medium in or on which the microorganism is cultured.

4.10.3 CYTOKINE AND CELL PROLIFERATION/DIFFERENTIATION ACTIVITY

A polypeptide of the present invention may exhibit activity relating to cytokine, cell proliferation (either inducing or inhibiting) or cell differentiation (either inducing or inhibiting) activity or may induce production of other cytokines in certain cell populations. A polypucleotide of the invention can encode a polypeptide exhibiting such attributes. Many protein factors discovered to date, including all known cytokines, have exhibited activity in one or more factor-dependent cell proliferation assays, and hence the assays serve as a convenient confirmation of cytokine activity. The activity of therapeutic compositions of the present invention is evidenced by any one of a number of routine factor dependent cell proliferation assays for cell lines including, without limitation, 32D, DA2, DA1G, T10, B9, B9/11, BaF3, MC9/G, M+(preB M+), 2E8, RB5, DA1, 123, T1165, HT2, CTLL2, TF-1, Mo7e, CMK, HUVEC, and Caco. Therapeutic compositions of the invention can be used in the following:

Assays for T-cell or thymocyte proliferation include without limitation those described in: Current Protocols in Immunology, Ed by J. E. Coligan, A. M. Kruisbeek, D. H. Margulies, E. M. Shevach, W. Strober, Pub. Greene Publishing Associates and Wiley-Interscience (Chapter 3, In Vitro assays for Mouse Lymphocyte Function 3.1-3.19; Chapter 7, Immunologic studies in Humans); Takai et al., J. Immunol. 137:3494-3500, 1986; Bertagnolli et al., J. Immunol. 145:1706-1712, 1990; Bertagnolli et al., Cellular Immunology 133:327-341, 1991; Bertagnolli, et al., I. Immunol. 149:3778-3783, 1992; Bowman et al., I. Immunol. 152:1756-1761, 1994.

Assays for cytokine production and/or proliferation of spleen cells, lymph node cells or thymocytes include, without limitation, those described in: Polyclonal T cell stimulation, Kruisbeek, A. M. and Shevach, E. M. In Current Protocols in Immunology. J. E. e.a. Coligan eds. Vol 1 pp. 3.12.1-3.12.14, John Wiley and Sons, Toronto. 1994; and Measurement of mouse and human interleukin- γ , Schreiber, R. D. In Current Protocols in Immunology. J. E. e.a. Coligan eds. Vol 1 pp. 6.8.1-6.8.8, John Wiley and Sons, Toronto. 1994.

Assays for proliferation and differentiation of hematopoietic and lymphopoietic cells include, without limitation, those described in: Measurement of Human and Murine Interleukin 2 and Interleukin 4, Bottomly, K., Davis, L. S. and Lipsky, P. E. In Current Protocols in Immunology. J. E. e.a. Coligan eds. Vol 1 pp. 6.3.1-6.3.12, John Wiley and Sons, Toronto. 1991; deVries et al., J. Exp. Med. 173:1205-1211, 1991; Moreau et al., Nature 336:690-692, 1988; Greenberger et al., Proc. Natl. Acad. Sci. U.S.A. 80:2931-2938, 1983; Measurement of mouse and human interleukin 6--Nordan, R. In Current Protocols in Immunology. J. E. Coligan eds. Vol 1 pp. 6.6.1-6.6.5, John Wiley and Sons, Toronto. 1991; Smith et al., Proc. Natl. Aced. Sci. U.S.A. 83:1857-1861, 1986; Measurement of human Interleukin 11--Bennett, F., Giannotti, J., Clark, S. C. and Turner, K. J. In Current Protocols in Immunology. J. E. Coligan eds. Vol 1 pp. 6.15.1 John Wiley and Sons, Toronto. 1991; Measurement of mouse and human Interleukin

9--Ciarletta, A., Giannotti, J., Clark, S. C. and Turner, K. J. In Current Protocols in Immunology.

J. E. Coligan eds. Vol 1 pp. 6.13.1. John Wiley and Sons. Toronto. 1991.

Assays for T-cell clone responses to antigens (which will identify, among others, proteins that affect APC-T cell interactions as well as direct T-cell effects by measuring proliferation and cytokine production) include, without limitation, those described in: Current Protocols in Immunology, Ed by J. E. Coligan, A. M. Kruisbeek, D. H. Margulies, E. M. Shevach, W Strober, Pub. Greene Publishing Associates and Wiley-Interscience (Chapter 3, *In Vitro* assays for Mouse Lymphocyte Function; Chapter 6, Cytokines and their cellular receptors; Chapter 7, Immunologic studies in Humans); Weinberger et al., Proc. Natl. Acad. Sci. USA 77:6091-6095, 1980; Weinberger et al., Eur. J. Immun. 11:405-411, 1981; Takai et al., J. Immunol. 137:3494-3500, 1986; Takai et al., J. Immunol. 140:508-512, 1988.

4.10.4 STEM CELL GROWTH FACTOR ACTIVITY

A polypeptide of the present invention may exhibit stem cell growth factor activity and be involved in the proliferation, differentiation and survival of pluripotent and totipotent stem cells including primordial germ cells, embryonic stem cells, hematopoietic stem cells and/or germ line stem cells. Administration of the polypeptide of the invention to stem cells in vivo or ex vivo is expected to maintain and expand cell populations in a totipotential or pluripotential state which would be useful for re-engineering damaged or diseased tissues, transplantation, manufacture of bio-pharmaceuticals and the development of bio-sensors. The ability to produce large quantities of human cells has important working applications for the production of human proteins which currently must be obtained from non-human sources or donors, implantation of cells to treat diseases such as Parkinson's, Alzheimer's and other neurodegenerative diseases; tissues for grafting such as bone marrow, skin, cartilage, tendons, bone, muscle (including cardiac muscle), blood vessels, cornea, neural cells, gastrointestinal cells and others; and organs for transplantation such as kidney, liver, pancreas (including islet cells), heart and lung.

It is contemplated that multiple different exogenous growth factors and/or cytokines may be administered in combination with the polypeptide of the invention to achieve the desired effect, including any of the growth factors listed herein, other stem cell maintenance factors, and specifically including stem cell factor (SCF), leukemia inhibitory factor (LIF), Flt-3 ligand (Flt-3L), any of the interleukins, recombinant soluble IL-6 receptor fused to IL-6, macrophage inflammatory protein 1-alpha (MIP-1-alpha), G-CSF, GM-CSF, thrombopoietin (TPO), platelet factor 4 (PF-4), platelet-derived growth factor (PDGF), neural growth factors and basic fibroblast growth factor (bFGF).

Since totipotent stem cells can give rise to virtually any mature cell type, expansion of these cells in culture will facilitate the production of large quantities of mature cells. Techniques for culturing stem cells are known in the art and administration of polypeptides of the invention, optionally with other growth factors and/or cytokines, is expected to enhance the survival and proliferation of the stem cell populations. This can be accomplished by direct administration of the polypeptide of the invention to the culture medium. Alternatively, stroma cells transfected with a polynucleotide that encodes for the polypeptide of the invention can be used as a feeder layer for the stem cell populations in culture or in vivo. Stromal support cells for feeder layers may include embryonic bone marrow fibroblasts, bone marrow stromal cells, fetal liver cells, or cultured embryonic fibroblasts (see U.S. Patent No. 5.690.926).

Stem cells themselves can be transfected with a polynucleotide of the invention to induce autocrine expression of the polypeptide of the invention. This will allow for generation of undifferentiated totipotential/pluripotential stem cell lines that are useful as is or that can then be differentiated into the desired mature cell types. These stable cell lines can also serve as a source of undifferentiated totipotential/pluripotential mRNA to create cDNA libraries and templates for polymerase chain reaction experiments. These studies would allow for the isolation and identification of differentially expressed genes in stem cell populations that regulate stem cell proliferation and/or maintenance.

Expansion and maintenance of totipotent stem cell populations will be useful in the treatment of many pathological conditions. For example, polypeptides of the present invention may be used to manipulate stem cells in culture to give rise to neuroepithelial cells that can be used to augment or replace cells damaged by illness, autoimmune disease, accidental damage or genetic disorders. The polypeptide of the invention may be useful for inducing the proliferation of neural cells and for the regeneration of nerve and brain tissue, i.e. for the treatment of central and peripheral nervous system diseases and neuropathies, as well as mechanical and traumatic disorders which involve degeneration, death or trauma to neural cells or nerve tissue. In addition, the expanded stem cell populations can also be genetically altered for gene therapy purposes and to decrease host rejection of replacement tissues after grafting or implantation.

Expression of the polypeptide of the invention and its effect on stem cells can also be manipulated to achieve controlled differentiation of the stem cells into more differentiated cell types. A broadly applicable method of obtaining pure populations of a specific differentiated cell type from undifferentiated stem cell populations involves the use of a cell-type specific promoter driving a selectable marker. The selectable marker allows only cells of the desired type to survive. For example, stem cells can be induced to differentiate into cardiomyocytes (Wobus et al., Differentiation, 48: 173-182, (1991); Klug et al., J. Clin. Invest., 98(1): 216-224, (1998))

or skeletal muscle cells (Browder, L. W. In: Principles of Tissue Engineering eds. Lanza et al., Academic Press (1997)). Alternatively, directed differentiation of stem cells can be accomplished by culturing the stem cells in the presence of a differentiation factor such as retinoic acid and an antagonist of the polypeptide of the invention which would inhibit the effects of endogenous stem cell factor activity and allow differentiation to proceed.

In vitro cultures of stem cells can be used to determine if the polypeptide of the invention exhibits stem cell growth factor activity. Stem cells are isolated from any one of various cell sources (including hematopoietic stem cells and embryonic stem cells) and cultured on a feeder layer, as described by Thompson et al. Proc. Natl. Acad. Sci., U.S.A., 92: 7844-7848 (1995), in the presence of the polypeptide of the invention alone or in combination with other growth factors or cytokines. The ability of the polypeptide of the invention to induce stem cells proliferation is determined by colony formation on semi-solid support e.g. as described by Bernstein et al., Blood, 77: 2316-2321 (1991).

4.10.5 HEMATOPOIESIS REGULATING ACTIVITY

A polypeptide of the present invention may be involved in regulation of hematopoiesis and, consequently, in the treatment of myeloid or lymphoid cell disorders. Even marginal biological activity in support of colony forming cells or of factor-dependent cell lines indicates involvement in regulating hematopoiesis, e.g. in supporting the growth and proliferation of erythroid progenitor cells alone or in combination with other cytokines, thereby indicating utility, for example, in treating various anemias or for use in conjunction with irradiation/chemotherapy to stimulate the production of erythroid precursors and/or erythroid cells; in supporting the growth and proliferation of myeloid cells such as granulocytes and monocytes/macrophages (i.e., traditional CSF activity) useful, for example, in conjunction with chemotherapy to prevent or treat consequent myelo-suppression; in supporting the growth and proliferation of megakaryocytes and consequently of platelets thereby allowing prevention or treatment of various platelet disorders such as thrombocytopenia, and generally for use in place of or complimentary to platelet transfusions; and/or in supporting the growth and proliferation of hematopoietic stem cells which are capable of maturing to any and all of the above-mentioned hematopoietic cells and therefore find therapeutic utility in various stem cell disorders (such as those usually treated with transplantation, including, without limitation, aplastic anemia and paroxysmal nocturnal hemoglobinuria), as well as in repopulating the stem cell compartment post irradiation/chemotherapy, either in-vivo or ex-vivo (i.e., in conjunction with bone marrow transplantation or with peripheral progenitor cell transplantation (homologous or heterologous)) as normal cells or genetically manipulated for gene therapy.

Therapeutic compositions of the invention can be used in the following:

Suitable assays for proliferation and differentiation of various hematopoietic lines are
cited above.

Assays for embryonic stem cell differentiation (which will identify, among others, proteins that influence embryonic differentiation hematopoiesis) include, without limitation, those described in: Johansson et al. Cellular Biology 15:141-151, 1995; Keller et al., Molecular and Cellular Biology 13:473-486, 1993; McClanahan et al., Blood 81:2903-2915, 1993.

Assays for stem cell survival and differentiation (which will identify, among others, proteins that regulate lympho-hematopoiesis) include, without limitation, those described in: Methylcellulose colony forming assays, Freshney, M. G. In Culture of Hematopoietic Cells. R. I. Freshney, et al. eds. Vol pp. 265-268, Wiley-Liss, Inc., New York, N.Y. 1994; Hirayama et al., Proc. Natl. Acad. Sci. USA 89:5907-5911, 1992; Primitive hematopoietic colony forming cells with high proliferative potential, McNiece, I. K. and Briddell, R. A. In Culture of Hematopoietic Cells. R. I. Freshney, et al. eds. Vol pp. 23-39, Wiley-Liss, Inc., New York, N.Y. 1994; Neben et al., Experimental Hematology 22:353-359, 1994; Cobblestone area forming cell assay, Ploemacher, R. E. In Culture of Hematopoietic Cells. R. I. Freshney, et al. eds. Vol pp. 1-21, Wiley-Liss, Inc., New York, N.Y. 1994; Long term bone marrow cultures in the presence of stromal cells, Spooncer, E., Dexter, M. and Allen, T. In Culture of Hematopoietic Cells. R. I. Freshney, et al. eds. Vol pp. 163-179, Wiley-Liss, Inc., New York, N.Y. 1994; Long term culture initiating cell assay, Sutherland, H. J. In Culture of Hematopoietic Cells. R. I. Freshney, et al. eds. Vol pp. 139-162, Wiley-Liss, Inc., New York, N.Y. 1994.

4.10.6 TISSUE GROWTH ACTIVITY

A polypeptide of the present invention also may be involved in bone, cartilage, tendon, ligament and/or nerve tissue growth or regeneration, as well as in wound healing and tissue repair and replacement, and in healing of burns, incisions and ulcers.

A polypeptide of the present invention which induces cartilage and/or bone growth in circumstances where bone is not normally formed, has application in the healing of bone fractures and cartilage damage or defects in humans and other animals. Compositions of a polypeptide, antibody, binding partner, or other modulator of the invention may have prophylactic use in closed as well as open fracture reduction and also in the improved fixation of artificial joints. De novo bone formation induced by an osteogenic agent contributes to the repair of congenital, trauma induced, or oncologic resection induced craniofacial defects, and also is useful in cosmetic plastic surgery.

A polypeptide of this invention may also be involved in attracting bone-forming cells, stimulating growth of bone-forming cells, or inducing differentiation of progenitors of bone-forming cells. Treatment of osteoporosis, osteoarthritis, bone degenerative disorders, or periodontal disease, such as through stimulation of bone and/or cartilage repair or by blocking inflammation or processes of tissue destruction (collagenase activity, osteoclast activity, etc.) mediated by inflammatory processes may also be possible using the composition of the invention.

Another category of tissue regeneration activity that may involve the polypeptide of the present invention is tendon/ligament formation. Induction of tendon/ligament-like tissue or other tissue formation in circumstances where such tissue is not normally formed, has application in the healing of tendon or ligament tears, deformities and other tendon or ligament defects in humans and other animals. Such a preparation employing a tendon/ligament-like tissue inducing protein may have prophylactic use in preventing damage to tendon or ligament tissue, as well as use in the improved fixation of tendon or ligament to bone or other tissues, and in repairing defects to tendon or ligament tissue. De novo tendon/ligament-like tissue formation induced by a composition of the present invention contributes to the repair of congenital, trauma induced, or other tendon or ligament defects of other origin, and is also useful in cosmetic plastic surgery for attachment or repair of tendons or ligaments. The compositions of the present invention may provide environment to attract tendon- or ligament-forming cells, stimulate growth of tendon- or ligament-forming cells, induce differentiation of progenitors of tendon- or ligament-forming cells, or induce growth of tendon/ligament cells or progenitors ex vivo for return in vivo to effect tissue repair. The compositions of the invention may also be useful in the treatment of tendinitis, carpal tunnel syndrome and other tendon or ligament defects. The compositions may also include an appropriate matrix and/or sequestering agent as a carrier as is well known in the art.

The compositions of the present invention may also be useful for proliferation of neural cells and for regeneration of nerve and brain tissue, i.e. for the treatment of central and peripheral nervous system diseases and neuropathies, as well as mechanical and traumatic disorders, which involve degeneration, death or trauma to neural cells or nerve tissue. More specifically, a composition may be used in the treatment of diseases of the peripheral nervous system, such as peripheral nerve injuries, peripheral neuropathy and localized neuropathies, and central nervous system diseases, such as Alzheimer's, Parkinson's disease, Huntington's disease, amyotrophic lateral sclerosis, and Shy-Drager syndrome. Further conditions which may be treated in accordance with the present invention include mechanical and traumatic disorders, such as spinal cord disorders, head trauma and cerebrovascular diseases such as stroke. Peripheral neuropathies

resulting from chemotherapy or other medical therapies may also be treatable using a composition of the invention.

Compositions of the invention may also be useful to promote better or faster closure of non-healing wounds, including without limitation pressure ulcers, ulcers associated with vascular insufficiency, surgical and traumatic wounds, and the like.

Compositions of the present invention may also be involved in the generation or regeneration of other tissues, such as organs (including, for example, pancreas, liver, intestine, kidney, skin, endothelium), muscle (smooth, skeletal or cardiac) and vascular (including vascular endothelium) tissue, or for promoting the growth of cells comprising such tissues. Part of the desired effects may be by inhibition or modulation of fibrotic scarring may allow normal tissue to regenerate. A polypeptide of the present invention may also exhibit angiogenic activity.

A composition of the present invention may also be useful for gut protection or regeneration and treatment of lung or liver fibrosis, reperfusion injury in various tissues, and conditions resulting from systemic cytokine damage.

A composition of the present invention may also be useful for promoting or inhibiting differentiation of tissues described above from precursor tissues or cells; or for inhibiting the growth of tissues described above.

Therapeutic compositions of the invention can be used in the following:

Assays for tissue generation activity include, without limitation, those described in: International Patent Publication No. WO95/16035 (bone, cartilage, tendon); International Patent Publication No. WO95/05846 (nerve, neuronal); International Patent Publication No. WO91/07491 (skin, endothelium).

Assays for wound healing activity include, without limitation, those described in: Winter, Epidermal Wound Healing, pps. 71-112 (Maibach, H. I. and Rovee, D. T., eds.), Year Book Medical Publishers, Inc., Chicago, as modified by Eaglstein and Mertz, J. Invest. Dermatol 71:382-84 (1978).

4.10.7 IMMUNE STIMULATING OR SUPPRESSING ACTIVITY

A polypeptide of the present invention may also exhibit immune stimulating or immune suppressing activity, including without limitation the activities for which assays are described herein. A polynucleotide of the invention can encode a polypeptide exhibiting such activities. A protein may be useful in the treatment of various immune deficiencies and disorders (including severe combined immunodeficiency (SCID)), e.g., in regulating (up or down) growth and proliferation of T and/or B lymphocytes, as well as effecting the cytolytic activity of NK cells and other cell populations. These immune deficiencies may be genetic or be caused by viral (e.g.,

HIV) as well as bacterial or fungal infections, or may result from autoimmune disorders. More specifically, infectious diseases causes by viral, bacterial, fungal or other infection may be treatable using a protein of the present invention, including infections by HIV, hepatitis viruses, herpes viruses, mycobacteria, Leishmania spp., malaria spp. and various fungal infections such as candidiasis. Of course, in this regard, proteins of the present invention may also be useful where a boost to the immune system generally may be desirable, i.e., in the treatment of cancer.

Autoimmune disorders which may be treated using a protein of the present invention include, for example, connective tissue disease, multiple sclerosis, systemic lupus erythematosus, rheumatoid arthritis, autoimmune pulmonary inflammation, Guillain-Barre syndrome, autoimmune thyroiditis, insulin dependent diabetes mellitis, myasthenia gravis, graft-versus-host disease and autoimmune inflammatory eye disease. Such a protein (or antagonists thereof, including antibodies) of the present invention may also to be useful in the treatment of allergic reactions and conditions (e.g., anaphylaxis, serum sickness, drug reactions, food allergies, insect venom allergies, mastocytosis, allergic rhinitis, hypersensitivity pneumonitis, urticaria, angioedema, eczema, atopic dermatitis, allergic contact dermatitis, erythema multiforme, Stevens-Johnson syndrome, allergic conjunctivitis, atopic keratoconjunctivitis, venereal keratoconjunctivitis, giant papillary conjunctivitis and contact allergies), such as asthma (particularly allergic asthma) or other respiratory problems. Other conditions, in which immune suppression is desired (including, for example, organ transplantation), may also be treatable using a protein (or antagonists thereof) of the present invention. The therapeutic effects of the polypeptides or antagonists thereof on allergic reactions can be evaluated by in vivo animals models such as the cumulative contact enhancement test (Lastborn et al., Toxicology 125: 59-66, 1998), skin prick test (Hoffmann et al., Allergy 54; 446-54, 1999), guinea pig skin sensitization test (Vohr et al., Arch. Toxocol. 73: 501-9), and murine local lymph node assay (Kimber et al., J. Toxicol. Environ. Health 53: 563-79).

Using the proteins of the invention it may also be possible to modulate immune responses, in a number of ways. Down regulation may be in the form of inhibiting or blocking an immune response already in progress or may involve preventing the induction of an immune response. The functions of activated T cells may be inhibited by suppressing T cell responses or by inducing specific tolerance in T cells, or both. Immunosuppression of T cell responses is generally an active, non-antigen-specific, process which requires continuous exposure of the T cells to the suppressive agent. Tolerance, which involves inducing non-responsiveness or anergy in T cells, is distinguishable from immunosuppression in that it is generally antigen-specific and persists after exposure to the tolerizing agent has ceased. Operationally, tolerance can be

demonstrated by the lack of a T cell response upon reexposure to specific antigen in the absence of the tolerizing agent.

Down regulating or preventing one or more antigen functions (including without limitation B lymphocyte antigen functions (such as, for example, B7)), e.g., preventing high level lymphokine synthesis by activated T cells, will be useful in situations of tissue, skin and organ transplantation and in graft-versus-host disease (GVHD). For example, blockage of T cell function should result in reduced tissue destruction in tissue transplantation. Typically, in tissue transplants, rejection of the transplant is initiated through its recognition as foreign by T cells, followed by an immune reaction that destroys the transplant. The administration of a therapeutic composition of the invention may prevent cytokine synthesis by immune cells, such as T cells, and thus acts as an immunosuppressant. Moreover, a lack of costimulation may also be sufficient to anergize the T cells, thereby inducing tolerance in a subject. Induction of long-term tolerance by B lymphocyte antigen-blocking reagents may avoid the necessity of repeated administration of these blocking reagents. To achieve sufficient immunosuppression or tolerance in a subject, it may also be necessary to block the function of a combination of B lymphocyte antigens.

The efficacy of particular therapeutic compositions in preventing organ transplant rejection or GVHD can be assessed using animal models that are predictive of efficacy in humans. Examples of appropriate systems which can be used include allogeneic cardiac grafts in rats and xenogeneic pancreatic islet cell grafts in mice, both of which have been used to examine the immunosuppressive effects of CTLA4Ig fusion proteins in vivo as described in Lenschow et al., Science 257:789-792 (1992) and Turka et al., Proc. Natl. Acad. Sci USA, 89:11102-11105 (1992). In addition, murine models of GVHD (see Paul ed., Fundamental Immunology, Raven Press, New York, 1989, pp. 846-847) can be used to determine the effect of therapeutic compositions of the invention on the development of that disease.

Blocking antigen function may also be therapeutically useful for treating autoimmune diseases. Many autoimmune disorders are the result of inappropriate activation of T cells that are reactive against self tissue and which promote the production of cytokines and autoantibodies involved in the pathology of the diseases. Preventing the activation of autoreactive T cells may reduce or eliminate disease symptoms. Administration of reagents which block stimulation of T cells can be used to inhibit T cell activation and prevent production of autoantibodies or T cell-derived cytokines which may be involved in the disease process. Additionally, blocking reagents may induce antigen-specific tolerance of autoreactive T cells which could lead to long-term relief from the disease. The efficacy of blocking reagents in preventing or alleviating autoimmune disorders can be determined using a number of well-characterized animal models of human autoimmune diseases. Examples include murine experimental autoimmune encephalitis,

systemic lupus erythmatosis in MRL/lpr/lpr mice or NZB hybrid mice, murine autoimmune collagen arthritis, diabetes mellitus in NOD mice and BB rats, and murine experimental myasthenia gravis (see Paul ed., Fundamental Immunology, Raven Press, New York, 1989, pp. 840-856).

Upregulation of an antigen function (e.g., a B lymphocyte antigen function), as a means of up regulating immune responses, may also be useful in therapy. Upregulation of immune responses may be in the form of enhancing an existing immune response or eliciting an initial immune response. For example, enhancing an immune response may be useful in cases of viral infection, including systemic viral diseases such as influenza, the common cold, and encephalitis.

Alternatively, anti-viral immune responses may be enhanced in an infected patient by removing T cells from the patient, costimulating the T cells in vitro with viral antigen-pulsed APCs either expressing a peptide of the present invention or together with a stimulatory form of a soluble peptide of the present invention and reintroducing the in vitro activated T cells into the patient. Another method of enhancing anti-viral immune responses would be to isolate infected cells from a patient, transfect them with a nucleic acid encoding a protein of the present invention as described herein such that the cells express all or a portion of the protein on their surface, and reintroduce the transfected cells into the patient. The infected cells would now be capable of delivering a costimulatory signal to, and thereby activate, T cells in vivo.

A polypeptide of the present invention may provide the necessary stimulation signal to T cells to induce a T cell mediated immune response against the transfected tumor cells. In addition, tumor cells which lack MHC class I or MHC class II molecules, or which fail to reexpress sufficient mounts of MHC class I or MHC class II molecules, can be transfected with nucleic acid encoding all or a portion of (e.g., a cytoplasmic-domain truncated portion) of an MHC class I alpha chain protein and β_2 microglobulin protein or an MHC class II alpha chain protein and an MHC class II beta chain protein to thereby express MHC class I or MHC class II proteins on the cell surface. Expression of the appropriate class I or class II MHC in conjunction with a peptide having the activity of a B lymphocyte antigen (e.g., B7-1, B7-2, B7-3) induces a T cell mediated immune response against the transfected tumor cell. Optionally, a gene encoding an antisense construct which blocks expression of an MHC class II associated protein, such as the invariant chain, can also be cotransfected with a DNA encoding a peptide having the activity of a B lymphocyte antigen to promote presentation of tumor associated antigens and induce tumor specific immunity. Thus, the induction of a T cell mediated immune response in a human subject may be sufficient to overcome tumor-specific tolerance in the subject.

The activity of a protein of the invention may, among other means, be measured by the following methods:

Suitable assays for thymocyte or splenocyte cytotoxicity include, without limitation, those described in: Current Protocols in Immunology, Ed by J. E. Coligan, A. M. Kruisbeek, D. H. Margulies, E. M. Shevach, W. Strober, Pub. Greene Publishing Associates and Wiley-Interscience (Chapter 3, In Vitro assays for Mouse Lymphocyte Function 3.1-3.19; Chapter 7, Immunologic studies in Humans); Herrmann et al., Proc. Natl. Acad. Sci. USA 78:2488-2492, 1981; Herrmann et al., J. Immunol. 128:1968-1974, 1982; Handa et al., J. Immunol. 135:1564-1572, 1985; Takai et al., I. Immunol. 137:3494-3500, 1986; Takai et al., J. Immunol. 140:508-512, 1988; Bowman et al., J. Virology 61:1992-1998; Bertagnolli et al., Cellular Immunology 133:327-341, 1991; Brown et al., J. Immunol. 153:3079-3092, 1994.

Assays for T-cell-dependent immunoglobulin responses and isotype switching (which will identify, among others, proteins that modulate T-cell dependent antibody responses and that affect Th1/Th2 profiles) include, without limitation, those described in: Maliszewski, J. Immunol. 144:3028-3033, 1990; and Assays for B cell function: In vitro antibody production, Mond, J. J. and Brunswick, M. In Current Protocols in Immunology. J. B. e.a. Coligan eds. Vol 1 pp. 3.8.1-3.8.16, John Wiley and Sons, Toronto. 1994.

Mixed lymphocyte reaction (MLR) assays (which will identify, among others, proteins that generate predominantly Th1 and CTL responses) include, without limitation, those described in: Current Protocols in Immunology, Ed by J. E. Coligan, A. M. Kruisbeek, D. H. Margulies, E. M. Shevach, W. Strober, Pub. Greene Publishing Associates and Wiley-Interscience (Chapter 3, In Vitro assays for Mouse Lymphocyte Function 3.1-3.19; Chapter 7, Immunologic studies in Humans); Takai et al., J. Immunol. 137:3494-3500, 1986; Takai et al., J. Immunol. 140:508-512, 1988; Bertagnolli et al., J. Immunol. 149:3778-3783, 1992.

Dendritic cell-dependent assays (which will identify, among others, proteins expressed by dendritic cells that activate naive T-cells) include, without limitation, those described in: Guery et al., J. Immunol. 134:536-544, 1995; Inaba et al., Journal of Experimental Medicine 173:549-559, 1991; Macatonia et al., Journal of Immunology 154:5071-5079, 1995; Porgador et al., Journal of Experimental Medicine 182:255-260, 1995; Nair et al., Journal of Virology 67:4062-4069, 1993; Huang et al., Science 264:961-965, 1994; Macatonia et al., Journal of Experimental Medicine 169:1255-1264, 1989; Bhardwaj et al., Journal of Clinical Investigation 94:797-807, 1994; and Inaba et al., Journal of Experimental Medicine 172:631-640, 1990.

Assays for lymphocyte survival/apoptosis (which will identify, among others, proteins that prevent apoptosis after superantigen induction and proteins that regulate lymphocyte homeostasis) include, without limitation, those described in: Darzynkiewicz et al., Cytometry

13:795-808, 1992; Gorczyca et al., Leukemia 7:659-670, 1993; Gorczyca et al., Cancer Research 53:1945-1951, 1993; Itoh et al., Cell 66:233-243, 1991; Zacharchuk, Journal of Immunology 145:4037-4045, 1990; Zamai et al., Cytometry 14:891-897, 1993; Gorczyca et al., International Journal of Oncology 1:639-648, 1992.

Assays for proteins that influence early steps of T-cell commitment and development include, without limitation, those described in: Antica et al., Blood 84:111-117, 1994; Fine et al., Cellular Immunology 155:111-122, 1994; Galy et al., Blood 85:2770-2778, 1995; Toki et al., Proc. Nat. Acad Sci. USA 88:7548-7551, 1991.

4.10.8 ACTIVIN/INHIBIN ACTIVITY

A polypeptide of the present invention may also exhibit activin- or inhibin-related activities. A polynucleotide of the invention may encode a polypeptide exhibiting such characteristics. Inhibins are characterized by their ability to inhibit the release of follicle stimulating hormone (FSH), while activins and are characterized by their ability to stimulate the release of follicle stimulating hormone (FSH). Thus, a polypeptide of the present invention, alone or in heterodimers with a member of the inhibin family, may be useful as a contraceptive based on the ability of inhibins to decrease fertility in female mammals and decrease spermatogenesis in male mammals. Administration of sufficient amounts of other inhibins can induce infertility in these mammals. Alternatively, the polypeptide of the invention, as a homodimer or as a heterodimer with other protein subunits of the inhibin group, may be useful as a fertility inducing therapeutic, based upon the ability of activin molecules in stimulating FSH release from cells of the anterior pituitary. See, for example, U.S. Pat. No. 4,798,885. A polypeptide of the invention may also be useful for advancement of the onset of fertility in sexually immature mammals, so as to increase the lifetime reproductive performance of domestic animals such as, but not limited to, cows, sheep and pigs.

The activity of a polypeptide of the invention may, among other means, be measured by the following methods.

Assays for activin/inhibin activity include, without limitation, those described in: Vale et al., Endocrinology 91:562-572, 1972; Ling et al., Nature 321:779-782, 1986; Vale et al., Nature 321:776-779, 1986; Mason et al., Nature 318:659-663, 1985; Forage et al., Proc. Natl. Acad. Sci. USA 83:3091-3095, 1986.

4.10.9 CHEMOTACTIC/CHEMOKINETIC ACTIVITY

A polypeptide of the present invention may be involved in chemotactic or chemokinetic activity for mammalian cells, including, for example, monocytes, fibroblasts, neutrophils,

T-cells, mast cells, eosinophils, epithelial and/or endothelial cells. A polynucleotide of the invention can encode a polypeptide exhibiting such attributes. Chemotactic and chemokinetic receptor activation can be used to mobilize or attract a desired cell population to a desired site of action. Chemotactic or chemokinetic compositions (e.g. proteins, antibodies, binding partners, or modulators of the invention) provide particular advantages in treatment of wounds and other trauma to tissues, as well as in treatment of localized infections. For example, attraction of lymphocytes, monocytes or neutrophils to tumors or sites of infection may result in improved immune responses against the tumor or infecting agent.

A protein or peptide has chemotactic activity for a particular cell population if it can stimulate, directly or indirectly, the directed orientation or movement of such cell population. Preferably, the protein or peptide has the ability to directly stimulate directed movement of cells. Whether a particular protein has chemotactic activity for a population of cells can be readily determined by employing such protein or peptide in any known assay for cell chemotaxis.

Therapeutic compositions of the invention can be used in the following:

Assays for chemotactic activity (which will identify proteins that induce or prevent chemotaxis) consist of assays that measure the ability of a protein to induce the migration of cells across a membrane as well as the ability of a protein to induce the adhesion of one cell population to another cell population. Suitable assays for movement and adhesion include, without limitation, those described in: Current Protocols in Immunology, Ed by J. E. Coligan, A. M. Kruisbeek, D. H. Marguiles, E. M. Shevach, W. Strober, Pub. Greene Publishing Associates and Wiley-Interscience (Chapter 6.12, Measurement of alpha and beta Chemokines 6.12.1-6.12.28; Taub et al. J. Clin. Invest. 95:1370-1376, 1995; Lind et al. APMIS 103:140-146, 1995; Muller et al Eur. J. Immunol. 25:1744-1748; Gruber et al. J. of Immunol. 152:5860-5867, 1994: Johnston et al. J. of Immunol. 153:1762-1768, 1994.

4.10.10 HEMOSTATIC AND THROMBOLYTIC ACTIVITY

A polypeptide of the invention may also be involved in hemostasis or thrombolysis or thrombosis. A polynucleotide of the invention can encode a polypeptide exhibiting such attributes. Compositions may be useful in treatment of various coagulation disorders (including hereditary disorders, such as hemophilias) or to enhance coagulation and other hemostatic events in treating wounds resulting from trauma, surgery or other causes. A composition of the invention may also be useful for dissolving or inhibiting formation of thromboses and for treatment and prevention of conditions resulting therefrom (such as, for example, infarction of cardiac and central nervous system vessels (e.g., stroke).

Therapeutic compositions of the invention can be used in the following:

Assay for hemostatic and thrombolytic activity include, without limitation, those described in: Linet et al., J. Clin. Pharmacol. 26:131-140, 1986; Burdick et al., Thrombosis Res. 45:413-419, 1987; Humphrey et al., Fibrinolysis 5:71-79 (1991); Schaub, Prostaglandins 35:467-474, 1988.

4.10.11 CANCER DIAGNOSIS AND THERAPY

Polypeptides of the invention may be involved in cancer cell generation, proliferation or metastasis. Detection of the presence or amount of polynucleotides or polypeptides of the invention may be useful for the diagnosis and/or prognosis of one or more types of cancer. For example, the presence or increased expression of a polynucleotide/polypeptide of the invention may indicate a hereditary risk of cancer, a precancerous condition, or an ongoing malignancy. Conversely, a defect in the gene or absence of the polypeptide may be associated with a cancer condition. Identification of single nucleotide polymorphisms associated with cancer or a predisposition to cancer may also be useful for diagnosis or prognosis.

Cancer treatments promote tumor regression by inhibiting tumor cell proliferation. inhibiting angiogenesis (growth of new blood vessels that is necessary to support tumor growth) and/or prohibiting metastasis by reducing tumor cell motility or invasiveness. Theraneutic compositions of the invention may be effective in adult and pediatric oncology including in solid phase tumors/malignancies, locally advanced tumors, human soft tissue sarcomas, metastatic cancer, including lymphatic metastases, blood cell malignancies including multiple myeloma, acute and chronic leukemias, and lymphomas, head and neck cancers including mouth cancer. larynx cancer and thyroid cancer, lung cancers including small cell carcinoma and non-small cell cancers, breast cancers including small cell carcinoma and ductal carcinoma, gastrointestinal cancers including esophageal cancer, stomach cancer, colon cancer, colorectal cancer and polyps associated with colorectal neoplasia, pancreatic cancers, liver cancer, urologic cancers including bladder cancer and prostate cancer, malignancies of the female genital tract including ovarian carcinoma, uterine (including endometrial) cancers, and solid tumor in the ovarian follicle, kidney cancers including renal cell carcinoma, brain cancers including intrinsic brain tumors, neuroblastoma, astrocytic brain tumors, gliomas, metastatic tumor cell invasion in the central nervous system, bone cancers including osteomas, skin cancers including malignant melanoma, tumor progression of human skin keratinocytes, squamous cell carcinoma, basal cell carcinoma, hemangiopericytoma and Karposi's sarcoma.

Polypeptides, polynucleotides, or modulators of polypeptides of the invention (including inhibitors and stimulators of the biological activity of the polypeptide of the invention) may be administered to treat cancer. Therapeutic compositions can be administered in therapeutically

effective dosages alone or in combination with adjuvant cancer therapy such as surgery, chemotherapy, radiotherapy, thermotherapy, and laser therapy, and may provide a beneficial effect, e.g. reducing tumor size, slowing rate of tumor growth, inhibiting metastasis, or otherwise improving overall clinical condition, without necessarily eradicating the cancer.

The composition can also be administered in therapeutically effective amounts as a portion of an anti-cancer cocktail. An anti-cancer cocktail is a mixture of the polypeptide or modulator of the invention with one or more anti-cancer drugs in addition to a pharmaceutically acceptable carrier for delivery. The use of anti-cancer cocktails as a cancer treatment is routine. Anti-cancer drugs that are well known in the art and can be used as a treatment in combination with the polypeptide or modulator of the invention include: Actinomycin D, Aminoglutethimide, Asparaginase, Bleomycin, Busulfan, Carboplatin, Carmustine, Chlorambucil, Cisplatin (cis-DDP). Cyclophosphamide. Cytarabine HCl (Cytosine arabinoside). Dacarbazine, Dactinomycin, Daunorubicin HCl, Doxorubicin HCl, Estramustine phosphate sodium, Etoposide (V16-213), Floxuridine, 5-Fluorouracil (5-Fu), Flutamide, Hydroxyurea (hydroxycarbamide), Ifosfamide, Interferon Alpha-2a, Interferon Alpha-2b, Leuprolide acetate (LHRH-releasing factor analog), Lomustine, Mechlorethamine HCl (nitrogen mustard), Melphalan, Mercaptopurine, Mesna, Methotrexate (MTX), Mitomycin, Mitoxantrone HCl, Octreotide, Plicamycin, Procarbazine HCl. Streptozocin, Tamoxifen citrate, Thioguanine, Thiotepa, Vinblastine sulfate, Vincristine sulfate, Amsacrine, Azacitidine, Hexamethylmelamine, Interleukin-2, Mitoguazone, Pentostatin, Semustine, Teniposide, and Vindesine sulfate.

In addition, therapeutic compositions of the invention may be used for prophylactic treatment of cancer. There are hereditary conditions and/or environmental situations (e.g. exposure to carcinogens) known in the art that predispose an individual to developing cancers. Under these circumstances, it may be beneficial to treat these individuals with therapeutically effective doses of the polypeptide of the invention to reduce the risk of developing cancers.

In vitro models can be used to determine the effective doses of the polypeptide of the invention as a potential cancer treatment. These in vitro models include proliferation assays of cultured tumor cells, growth of cultured tumor cells in soft agar (see Freshney, (1987) Culture of Animal Cells: A Manual of Basic Technique, Wily-Liss, New York, NY Ch 18 and Ch 21), tumor systems in nude mice as described in Giovanella et al., J. Natl. Can. Inst., 52: 921-30 (1974), mobility and invasive potential of tumor cells in Boyden Chamber assays as described in Pilkington et al., Anticancer Res., 17: 4107-9 (1997), and angiogenesis assays such as induction of vascularization of the chick chorioallantoic membrane or induction of vascular endothelial cell migration as described in Ribatta et al., Intl. J. Dev. Biol., 40: 1189-97 (1999) and Li et al., Clin. Exp. Metastasis, 17:423-9 (1999), respectively. Suitable tumor cells lines are available,

e.g. from American Type Tissue Culture Collection catalogs.

4.10.12 RECEPTOR/LIGAND ACTIVITY

A polypeptide of the present invention may also demonstrate activity as receptor, receptor ligand or inhibitor or agonist of receptor/ligand interactions. A polynucleotide of the invention can encode a polypeptide exhibiting such characteristics. Examples of such receptors and ligands include, without limitation, cytokine receptors and their ligands, receptor phosphatases and their ligands, receptor involved in cell-cell interactions and their ligands (including without limitation, cellular adhesion molecules (such as selectins, integrins and their ligands) and receptor/ligand pairs involved in antigen presentation, antigen recognition and development of cellular and humoral immune responses. Receptors and ligands are also useful for screening of potential peptide or small molecule inhibitors of the relevant receptor/ligand interaction. A protein of the present invention (including, without limitation, fragments of receptors and ligands) may themselves be useful as inhibitors of receptor/ligand interactions.

The activity of a polypeptide of the invention may, among other means, be measured by the following methods:

Suitable assays for receptor-ligand activity include without limitation those described in: Current Protocols in Immunology, Ed by J. E. Coligan, A. M. Kruisbeek, D. H. Margulies, E. M. Shevach, W. Strober, Pub. Greene Publishing Associates and Wiley- Interscience (Chapter 7.28, Measurement of Cellular Adhesion under static conditions 7.28.1-7.28.22), Takai et al., Proc. Natl. Acad. Sci. USA 84:6864-6868, 1987; Bierer et al., J. Exp. Med. 168:1145-1156, 1988; Rosenstein et al., J. Exp. Med. 169:149-160 1989; Stoltenborg et al., J. Immunol. Methods 175:59-68, 1994; Stitt et al., Cell 80:661-670, 1995.

By way of example, the polypeptides of the invention may be used as a receptor for a ligand(s) thereby transmitting the biological activity of that ligand(s). Ligands may be identified through binding assays, affinity chromatography, dihybrid screening assays, BIAcore assays, gel overlay assays, or other methods known in the art.

Studies characterizing drugs or proteins as agonist or antagonist or partial agonists or a partial antagonist require the use of other proteins as competing ligands. The polypeptides of the present invention or ligand(s) thereof may be labeled by being coupled to radioisotopes, colorimetric molecules or a toxin molecules by conventional methods. ("Guide to Protein Purification" Murray P. Deutscher (ed) Methods in Enzymology Vol. 182 (1990) Academic Press, Inc. San Diego). Examples of radioisotopes include, but are not limited to, tritium and carbon-14. Examples of colorimetric molecules include, but are not limited to, fluorescent

molecules such as fluorescamine, or rhodamine or other colorimetric molecules. Examples of toxins include, but are not limited, to ricin.

4.10.13 DRUG SCREENING

This invention is particularly useful for screening chemical compounds by using the novel polypeptides or binding fragments thereof in any of a variety of drug screening techniques. The polypeptides or fragments employed in such a test may either be free in solution, affixed to a solid support, borne on a cell surface or located intracellularly. One method of drug screening utilizes eukaryotic or prokaryotic host cells which are stably transformed with recombinant nucleic acids expressing the polypeptide or a fragment thereof. Drugs are screened against such transformed cells in competitive binding assays. Such cells, either in viable or fixed form, can be used for standard binding assays. One may measure, for example, the formation of complexes between polypeptides of the invention or fragments and the agent being tested or examine the diminution in complex formation between the novel polypeptides and an appropriate cell line, which are well known in the art.

Sources for test compounds that may be screened for ability to bind to or modulate (i.e., increase or decrease) the activity of polypeptides of the invention include (1) inorganic and organic chemical libraries, (2) natural product libraries, and (3) combinatorial libraries comprised of either random or mimetic peptides, oligonucleotides or organic molecules.

Chemical libraries may be readily synthesized or purchased from a number of commercial sources, and may include structural analogs of known compounds or compounds that are identified as "hits" or "leads" via natural product screening.

The sources of natural product libraries are microorganisms (including bacteria and fungi), animals, plants or other vegetation, or marine organisms, and libraries of mixtures for screening may be created by: (1) fermentation and extraction of broths from soil, plant or marine microorganisms or (2) extraction of the organisms themselves. Natural product libraries include polyketides, non-ribosomal peptides, and (non-naturally occurring) variants thereof. For a review, see Science 282:63-68 (1998).

Combinatorial libraries are composed of large numbers of peptides, oligonucleotides or organic compounds and can be readily prepared by traditional automated synthesis methods, PCR, cloning or proprietary synthetic methods. Of particular interest are peptide and oligonucleotide combinatorial libraries. Still other libraries of interest include peptide, protein, peptidomimetic, multiparallel synthetic collection, recombinatorial, and polypeptide libraries. For a review of combinatorial chemistry and libraries created therefrom, see Myers, Curr. Opin. Biotechnol. 8:701-707 (1997). For reviews and examples of peptidomimetic libraries, see

Al-Obeidi et al., Mol. Biotechnol, 9(3):205-23 (1998); Hruby et al., Curr Opin Chem Biol, 1(1):114-19 (1997); Dorner et al., Bioorg Med Chem, 4(5):709-15 (1996) (alkylated dipeptides).

Identification of modulators through use of the various libraries described herein permits modification of the candidate "hit" (or "lead") to optimize the capacity of the "hit" to bind a polypeptide of the invention. The molecules identified in the binding assay are then tested for antagonist or agonist activity in in vivo tissue culture or animal models that are well known in the art. In brief, the molecules are titrated into a plurality of cell cultures or animals and then tested for either cell/animal death or prolonged survival of the animal/cells.

The binding molecules thus identified may be complexed with toxins, e.g., ricin or cholera, or with other compounds that are toxic to cells such as radioisotopes. The toxin-binding molecule complex is then targeted to a tumor or other cell by the specificity of the binding molecule for a polypeptide of the invention. Alternatively, the binding molecules may be complexed with imaging agents for targeting and imaging purposes.

4.10.14 ASSAY FOR RECEPTOR ACTIVITY

The invention also provides methods to detect specific binding of a polypeptide e.g. a ligand or a receptor. The art provides numerous assays particularly useful for identifying previously unknown binding partners for receptor polypeptides of the invention. For example, expression cloning using mammalian or bacterial cells, or dihybrid screening assays can be used to identify polynucleotides encoding binding partners. As another example, affinity chromatography with the appropriate immobilized polypeptide of the invention can be used to isolate polypeptides that recognize and bind polypeptides of the invention. There are a number of different libraries used for the identification of compounds, and in particular small molecules. that modulate (i.e., increase or decrease) biological activity of a polypeptide of the invention. Ligands for receptor polypeptides of the invention can also be identified by adding exogenous ligands, or cocktails of ligands to two cells populations that are genetically identical except for the expression of the receptor of the invention: one cell population expresses the receptor of the invention whereas the other does not. The response of the two cell populations to the addition of ligands(s) are then compared. Alternatively, an expression library can be co-expressed with the polypeptide of the invention in cells and assayed for an autocrine response to identify potential ligand(s). As still another example, BIAcore assays, gel overlay assays, or other methods known in the art can be used to identify binding partner polypeptides, including, (1) organic and inorganic chemical libraries, (2) natural product libraries, and (3) combinatorial libraries comprised of random pentides, oligonucleotides or organic molecules.

The role of downstream intracellular signaling molecules in the signaling cascade of the polypeptide of the invention can be determined. For example, a chimeric protein in which the cytoplasmic domain of the polypeptide of the invention is fused to the extracellular portion of a protein, whose ligand has been identified, is produced in a host cell. The cell is then incubated with the ligand specific for the extracellular portion of the chimeric protein, thereby activating the chimeric receptor. Known downstream proteins involved in intracellular signaling can then be assayed for expected modifications i.e. phosphorylation. Other methods known to those in the art can also be used to identify signaling molecules involved in receptor activity.

4.10.15 ANTI-INFLAMMATORY ACTIVITY

Compositions of the present invention may also exhibit anti-inflammatory activity. The anti-inflammatory activity may be achieved by providing a stimulus to cells involved in the inflammatory response, by inhibiting or promoting cell-cell interactions (such as, for example, cell adhesion), by inhibiting or promoting chemotaxis of cells involved in the inflammatory process, inhibiting or promoting cell extravasation, or by stimulating or suppressing production of other factors which more directly inhibit or promote an inflammatory response. Compositions with such activities can be used to treat inflammatory conditions including chronic or acute conditions), including without limitation intimation associated with infection (such as septic shock, sepsis or systemic inflammatory response syndrome (SIRS)), ischemia-reperfusion injury, endotoxin lethality, arthritis, complement-mediated hyperacute rejection, nephritis, cytokine or chemokine-induced lung injury, inflammatory bowel disease, Crohn's disease or resulting from over production of cytokines such as TNF or IL-1. Compositions of the invention may also be useful to treat anaphylaxis and hypersensitivity to an antigenic substance or material. Compositions of this invention may be utilized to prevent or treat conditions such as, but not limited to, sepsis, acute pancreatitis, endotoxin shock, cytokine induced shock, rheumatoid arthritis, chronic inflammatory arthritis, pancreatic cell damage from diabetes mellitus type 1, graft versus host disease, inflammatory bowel disease, inflamation associated with pulmonary disease, other autoimmune disease or inflammatory disease, an antiproliferative agent such as for acute or chronic mylegenous leukemia or in the prevention of premature labor secondary to intrauterine infections.

4.10.16 LEUKEMIAS

Leukemias and related disorders may be treated or prevented by administration of a therapeutic that promotes or inhibits function of the polynucleotides and/or polypeptides of the invention. Such leukemias and related disorders include but are not limited to acute leukemia, acute lymphocytic leukemia, acute myelocytic leukemia, myeloblastic, promyelocytic, myelomonocytic, monocytic, erythroleukemia, chronic leukemia, chronic myelocytic (granulocytic) leukemia and chronic lymphocytic leukemia (for a review of such disorders, see Fishman et al., 1985, Medicine, 2d Ed., J.B. Lippincott Co., Philadelphia).

4.10.17 NERVOUS SYSTEM DISORDERS

Nervous system disorders, involving cell types which can be tested for efficacy of intervention with compounds that modulate the activity of the polynucleotides and/or polypeptides of the invention, and which can be treated upon thus observing an indication of therapeutic utility, include but are not limited to nervous system injuries, and diseases or disorders which result in either a disconnection of axons, a diminution or degeneration of neurons, or demyelination. Nervous system lesions which may be treated in a patient (including human and non-human mammalian patients) according to the invention include but are not limited to the following lesions of either the central (including spinal cord, brain) or peripheral nervous systems:

- (i) traumatic lesions, including lesions caused by physical injury or associated with surgery, for example, lesions which sever a portion of the nervous system, or compression injuries;
- (ii) ischemic lesions, in which a lack of oxygen in a portion of the nervous system results in neuronal injury or death, including cerebral infarction or ischemia, or spinal cord infarction or ischemia;
- (iii) infectious lesions, in which a portion of the nervous system is destroyed or injured as a result of infection, for example, by an abscess or associated with infection by human immunodeficiency virus, herpes zoster, or herpes simplex virus or with Lyme disease, tuberculosis, syphilis;
- (iv) degenerative lesions, in which a portion of the nervous system is destroyed or injured as a result of a degenerative process including but not limited to degeneration associated with Parkinson's disease, Alzheimer's disease, Huntington's chorea, or amyotrophic lateral sclerosis;
- (v) lesions associated with nutritional diseases or disorders, in which a portion of the nervous system is destroyed or injured by a nutritional disorder or disorder of metabolism including but not limited to, vitamin B12 deficiency, folic acid deficiency, Wernicke disease, tobacco-alcohol amblyopia, Marchiafava-Bignami disease (primary degeneration of the corpus callosum), and alcoholic cerebellar degeneration;

- (vi) neurological lesions associated with systemic diseases including but not limited to diabetes (diabetic neuropathy, Bell's palsy), systemic lupus erythematosus, carcinoma, or sarcoidosis:
- (vii) lesions caused by toxic substances including alcohol, lead, or particular neurotoxins; and
- (viii) demyelinated lesions in which a portion of the nervous system is destroyed or injured by a demyelinating disease including but not limited to multiple sclerosis, human immunodeficiency virus-associated myelopathy, transverse myelopathy or various etiologies, progressive multifocal leukoencephalopathy, and central pontine myelinolysis.

Therapeutics which are useful according to the invention for treatment of a nervous system disorder may be selected by testing for biological activity in promoting the survival or differentiation of neurons. For example, and not by way of limitation, therapeutics which elicit any of the following effects may be useful according to the invention:

- (i) increased survival time of neurons in culture;
- (ii) increased sprouting of neurons in culture or in vivo;
- (iii) increased production of a neuron-associated molecule in culture or *in vivo*, e.g., choline acetyltransferase or acetylcholinesterase with respect to motor neurons; or
 - (iv) decreased symptoms of neuron dysfunction in vivo.

Such effects may be measured by any method known in the art. In preferred, non-limiting embodiments, increased survival of neurons may be measured by the method set forth in Arakawa et al. (1990, J. Neurosci. 10:3507-3515); increased sprouting of neurons may be detected by methods set forth in Pestronk et al. (1980, Exp. Neurol. 70:65-82) or Brown et al. (1981, Ann. Rev. Neurosci. 4:17-42); increased production of neuron-associated molecules may be measured by bioassay, enzymatic assay, antibody binding, Northern blot assay, etc., depending on the molecule to be measured; and motor neuron dysfunction may be measured by assessing the physical manifestation of motor neuron disorder, e.g., weakness, motor neuron conduction velocity, or functional disability.

In specific embodiments, motor neuron disorders that may be treated according to the invention include but are not limited to disorders such as infarction, infection, exposure to toxin, trauma, surgical damage, degenerative disease or malignancy that may affect motor neurons as well as other components of the nervous system, as well as disorders that selectively affect neurons such as amyotrophic lateral sclerosis, and including but not limited to progressive spinal muscular atrophy, progressive bulbar palsy, primary lateral sclerosis, infantile and juvenile muscular atrophy, progressive bulbar paralysis of childhood (Fazio-Londe syndrome),

poliomyelitis and the post polio syndrome, and Hereditary Motorsensory Neuropathy (Charcot-Marie-Tooth Disease).

4.10.18 OTHER ACTIVITIES

A polypeptide of the invention may also exhibit one or more of the following additional activities or effects; inhibiting the growth, infection or function of, or killing, infectious agents. including, without limitation, bacteria, viruses, fungi and other parasites; effecting (suppressing or enhancing) bodily characteristics, including, without limitation, height, weight, hair color, eye color, skin, fat to lean ratio or other tissue pigmentation, or organ or body part size or shape (such as, for example, breast augmentation or diminution, change in bone form or shape): effecting biorhythms or circadian cycles or rhythms; effecting the fertility of male or female subjects; effecting the metabolism, catabolism, anabolism, processing, utilization, storage or elimination of dietary fat, lipid, protein, carbohydrate, vitamins, minerals, co-factors or other nutritional factors or component(s); effecting behavioral characteristics, including, without limitation, appetite, libido, stress, cognition (including cognitive disorders), depression (including depressive disorders) and violent behaviors; providing analgesic effects or other pain reducing effects; promoting differentiation and growth of embryonic stem cells in lineages other than hematopoietic lineages; hormonal or endocrine activity; in the case of enzymes, correcting deficiencies of the enzyme and treating deficiency-related diseases; treatment of hyperproliferative disorders (such as, for example, psoriasis); immunoglobulin-like activity (such as, for example, the ability to bind antigens or complement); and the ability to act as an antigen in a vaccine composition to raise an immune response against such protein or another material or entity which is cross-reactive with such protein.

4.10.19 IDENTIFICATION OF POLYMORPHISMS

The demonstration of polymorphisms makes possible the identification of such polymorphisms in human subjects and the pharmacogenetic use of this information for diagnosis and treatment. Such polymorphisms may be associated with, e.g., differential predisposition or susceptibility to various disease states (such as disorders involving inflammation or immune response) or a differential response to drug administration, and this genetic information can be used to tailor preventive or therapeutic treatment appropriately. For example, the existence of a polymorphism associated with a predisposition to inflammation or autoimmune disease makes possible the diagnosis of this condition in humans by identifying the presence of the polymorphism.

Polymorphisms can be identified in a variety of ways known in the art which all generally involve obtaining a sample from a patient, analyzing DNA from the sample, optionally involving isolation or amplification of the DNA, and identifying the presence of the polymorphism in the DNA. For example, PCR may be used to amplify an appropriate fragment of genomic DNA which may then be sequenced. Alternatively, the DNA may be subjected to allele-specific oligonucleotide hybridization (in which appropriate oligonucleotides are hybridized to the DNA under conditions permitting detection of a single base mismatch) or to a single nucleotide extension assay (in which an oligonucleotide that hybridizes immediately adjacent to the position of the polymorphism is extended with one or more labeled nucleotides). In addition, traditional restriction fragment length polymorphism analysis (using restriction enzymes that provide differential digestion of the genomic DNA depending on the presence or absence of the polymorphism) may be performed. Arrays with nucleotide sequences of the present invention can be used to detect polymorphisms. The array can comprise modified nucleotide sequences of the present invention in order to detect the nucleotide sequences of the present invention. In the alternative, any one of the nucleotide sequences of the present invention can be placed on the array to detect changes from those sequences.

Alternatively a polymorphism resulting in a change in the amino acid sequence could also be detected by detecting a corresponding change in amino acid sequence of the protein, e.g., by an antibody specific to the variant sequence.

4.10.20 ARTHRITIS AND INFLAMMATION

The immunosuppressive effects of the compositions of the invention against rheumatoid arthritis is determined in an experimental animal model system. The experimental model system is adjuvant induced arthritis in rats, and the protocol is described by J. Holoshitz, et at., 1983, Science, 219:56, or by B. Waksman et al., 1963, Int. Arch. Allergy Appl. Immunol., 23:129. Induction of the disease can be caused by a single injection, generally intradermally, of a suspension of killed Mycobacterium tuberculosis in complete Freund's adjuvant (CFA). The route of injection can vary, but rats may be injected at the base of the tail with an adjuvant mixture. The polypeptide is administered in phosphate buffered solution (PBS) at a dose of about 1-5 mg/kg. The control consists of administering PBS only.

The procedure for testing the effects of the test compound would consist of intradermally injecting killed Mycobacterium tuberculosis in CFA followed by immediately administering the test compound and subsequent treatment every other day until day 24. At 14, 15, 18, 20, 22, and 24 days after injection of Mycobacterium CFA, an overall arthritis score may be obtained as described by J. Holoskitz above. An analysis of the data would reveal that the test compound

would have a dramatic affect on the swelling of the joints as measured by a decrease of the

4.11 THERAPEUTIC METHODS :

The compositions (including polypeptide fragments, analogs, variants and antibodies or other binding partners or modulators including antisense polynucleotides) of the invention have numerous applications in a variety of therapeutic methods. Examples of therapeutic applications include, but are not limited to, those exemplified herein.

4.11.1 EXAMPLE

One embodiment of the invention is the administration of an effective amount of the polypeptides or other composition of the invention to individuals affected by a disease or disorder that can be modulated by regulating the peptides of the invention. While the mode of administration is not particularly important, parenteral administration is preferred. An exemplary mode of administration is to deliver an intravenous bolus. The dosage of the polypeptides or other composition of the invention will normally be determined by the prescribing physician. It is to be expected that the dosage will vary according to the age, weight. condition and response of the individual patient. Typically, the amount of polypeptide administered per dose will be in the range of about 0.01µg/kg to 100 mg/kg of body weight, with the preferred dose being about 0.1µg/kg to 10 mg/kg of patient body weight. For parenteral administration, polypeptides of the invention will be formulated in an injectable form combined with a pharmaceutically acceptable parenteral vehicle. Such vehicles are well known in the art and examples include water, saline, Ringer's solution, dextrose solution, and solutions consisting of small amounts of the human serum albumin. The vehicle may contain minor amounts of additives that maintain the isotonicity and stability of the polypeptide or other active ingredient. The preparation of such solutions is within the skill of the art.

4.12 PHARMACEUTICAL FORMULATIONS AND ROUTES OF ADMINISTRATION

A protein or other composition of the present invention (from whatever source derived, including without limitation from recombinant and non-recombinant sources and including antibodies and other binding partners of the polypeptides of the invention) may be administered to a patient in need, by itself, or in pharmaceutical compositions where it is mixed with suitable carriers or excipient(s) at doses to treat or ameliorate a variety of disorders. Such a composition may optionally contain (in addition to protein or other active ingredient and a carrier) diluents,

fillers, salts, buffers, stabilizers, solubilizers, and other materials well known in the art. The term "pharmaceutically acceptable" means a non-toxic material that does not interfere with the effectiveness of the biological activity of the active ingredient(s). The characteristics of the carrier will depend on the route of administration. The pharmaceutical composition of the invention may also contain cytokines, lymphokines, or other hematopoietic factors such as M-CSF, GM-CSF, TNF, IL-1, IL-2, IL-3, IL-4, IL-5, IL-6, IL-7, IL-8, IL-9, IL-10, IL-11, IL-12, IL-13, IL-14, IL-15, IFN, TNF0, TNF1, TNF2, G-CSF, Meg-CSF, thrombopoietin, stem cell factor, and erythropoietin. In further compositions, proteins of the invention may be combined with other agents beneficial to the treatment of the disease or disorder in question. These agents include various growth factors such as epidermal growth factor (EGF), platelet-derived growth factor (PDGF), transforming growth factors (TGF-α and TGF-β), insulin-like growth factor (IGF), as well as cytokines described herein.

The pharmaceutical composition may further contain other agents which either enhance the activity of the protein or other active ingredient or complement its activity or use in treatment. Such additional factors and/or agents may be included in the pharmaceutical composition to produce a synergistic effect with protein or other active ingredient of the invention, or to minimize side effects. Conversely, protein or other active ingredient of the present invention may be included in formulations of the particular clotting factor, cytokine, lymphokine, other hematopoietic factor, thrombolytic or anti-thrombotic factor, or anti-inflammatory agent to minimize side effects of the clotting factor, cytokine, lymphokine, other hematopoietic factor, thrombolytic or anti-thrombotic factor, cytokine, other hematopoietic factor, thrombolytic or anti-thrombotic factor, or anti-inflammatory agent (such as IL-1Ra, IL-1 Hy1, IL-1 Hy2, anti-TNF, corticosteroids, immunosuppressive agents). A protein of the present invention may be active in multimers (e.g., heterodimers or homodimers) or complexes with itself or other proteins. As a result, pharmaceutical compositions of the invention may comprise a protein of the invention in such multimeric or complexed form.

As an alternative to being included in a pharmaceutical composition of the invention including a first protein, a second protein or a therapeutic agent may be concurrently administered with the first protein (e.g., at the same time, or at differing times provided that therapeutic concentrations of the combination of agents is achieved at the treatment site). Techniques for formulation and administration of the compounds of the instant application may be found in "Remington's Pharmaceutical Sciences," Mack Publishing Co., Easton, PA, latest edition. A therapeutically effective dose further refers to that amount of the compound sufficient to result in amelioration of symptoms, e.g., treatment, healing, prevention or amelioration of the relevant medical condition, or an increase in rate of treatment, healing, prevention or amelioration of such conditions. When applied to an individual active ingredient, administered

alone, a therapeutically effective dose refers to that ingredient alone. When applied to a combination, a therapeutically effective dose refers to combined amounts of the active ingredients that result in the therapeutic effect, whether administered in combination, serially or simultaneously.

In practicing the method of treatment or use of the present invention, a therapeutically effective amount of protein or other active ingredient of the present invention is administered to a mammal having a condition to be treated. Protein or other active ingredient of the present invention may be administered in accordance with the method of the invention either alone or in combination with other therapies such as treatments employing cytokines, lymphokines or other hematopoietic factors. When co- administered with one or more cytokines, lymphokines or other hematopoietic factors, protein or other active ingredient of the present invention may be administered either simultaneously with the cytokine(s), lymphokine(s), other hematopoietic factors(s), thrombolytic or anti-thrombotic factors, or sequentially. If administered sequentially, the attending physician will decide on the appropriate sequence of administering protein or other active ingredient of the present invention in combination with cytokine(s), lymphokine(s), other hematopoietic factors(s), thrombolytic or anti-thrombotic factors.

4.12.1 ROUTES OF ADMINISTRATION

Suitable routes of administration may, for example, include oral, rectal, transmucosal, or intestinal administration; parenteral delivery, including intramuscular, subcutaneous, intramedullary injections, as well as intrathecal, direct intraventricular, intravenous, intraperitoneal, intranasal, or intraocular injections. Administration of protein or other active ingredient of the present invention used in the pharmaceutical composition or to practice the method of the present invention can be carried out in a variety of conventional ways, such as oral ingestion, inhalation, topical application or cutaneous, subcutaneous, intraperitoneal, parenteral or intravenous injection. Intravenous administration to the patient is preferred.

Alternately, one may administer the compound in a local rather than systemic manner, for example, via injection of the compound directly into a arthritic joints or in fibrotic tissue, often in a depot or sustained release formulation. In order to prevent the scarring process frequently occurring as complication of glaucoma surgery, the compounds may be administered topically, for example, as eye drops. Furthermore, one may administer the drug in a targeted drug delivery system, for example, in a liposome coated with a specific antibody, targeting, for example, arthritic or fibrotic tissue. The liposomes will be targeted to and taken up selectively by the afflicted tissue.

The polypeptides of the invention are administered by any route that delivers an effective dosage to the desired site of action. The determination of a suitable route of administration and an effective dosage for a particular indication is within the level of skill in the art. Preferably for wound treatment, one administers the therapeutic compound directly to the site. Suitable dosage ranges for the polypeptides of the invention can be extrapolated from these dosages or from similar studies in appropriate animal models. Dosages can then be adjusted as necessary by the clinician to provide maximal therapeutic benefit.

4.12.2 COMPOSITIONS/FORMULATIONS

Pharmaceutical compositions for use in accordance with the present invention thus may be formulated in a conventional manner using one or more physiologically acceptable carriers comprising excipients and auxiliaries which facilitate processing of the active compounds into preparations which can be used pharmaceutically. These pharmaceutical compositions may be manufactured in a manner that is itself known, e.g., by means of conventional mixing, dissolving, granulating, draggee-making, levigating, emulsifying, encapsulating, entrapping or lyophilizing processes. Proper formulation is dependent upon the route of administration chosen. When a therapeutically effective amount of protein or other active ingredient of the present invention is administered orally, protein or other active ingredient of the present Invention will be in the form of a tablet, capsule, powder, solution or elixir. When administered in tablet form, the pharmaceutical composition of the invention may additionally contain a solid carrier such as a gelatin or an adjuvant. The tablet, capsule, and powder contain from about 5 to 95% protein or other active ingredient of the present invention, and preferably from about 25 to 90% protein or other active ingredient of the present invention. When administered in liquid form, a liquid carrier such as water, petroleum, oils of animal or plant origin such as peanut oil. mineral oil, soybean oil, or sesame oil, or synthetic oils may be added. The liquid form of the pharmaceutical composition may further contain physiological saline solution, dextrose or other saccharide solution, or glycols such as ethylene glycol, propylene glycol or polyethylene glycol. When administered in liquid form, the pharmaceutical composition contains from about 0.5 to 90% by weight of protein or other active ingredient of the present invention, and preferably from about 1 to 50% protein or other active ingredient of the present invention.

When a therapeutically effective amount of protein or other active ingredient of the present invention is administered by intravenous, cutaneous or subcutaneous injection, protein or other active ingredient of the present invention will be in the form of a pyrogen-free, parenterally acceptable aqueous solution. The preparation of such parenterally acceptable protein or other active ingredient solutions, having due regard to pH, isotonicity, stability, and the like, is within

the skill in the art. A preferred pharmaceutical composition for intravenous, cutaneous, or subcutaneous injection should contain, in addition to protein or other active ingredient of the present invention, an isotonic vehicle such as Sodium Chloride Injection, Ringer's Injection, Dextrose Injection, Dextrose and Sodium Chloride Injection, Lactated Ringer's Injection, or other vehicle as known in the art. The pharmaceutical composition of the present invention may also contain stabilizers, preservatives, buffers, antioxidants, or other additives known to those of skill in the art. For injection, the agents of the invention may be formulated in aqueous solutions, preferably in physiologically compatible buffers such as Hanks's solution, Ringer's solution, or physiological saline buffer. For transmucosal administration, penetrants appropriate to the barrier to be permeated are used in the formulation. Such penetrants are generally known in the art.

For oral administration, the compounds can be formulated readily by combining the active compounds with pharmaceutically acceptable carriers well known in the art. Such carriers enable the compounds of the invention to be formulated as tablets, pills, dragees, capsules. liquids, gels, syrups, slurries, suspensions and the like, for oral ingestion by a patient to be treated. Pharmaceutical preparations for oral use can be obtained from a solid excipient. optionally grinding a resulting mixture, and processing the mixture of granules, after adding suitable auxiliaries, if desired, to obtain tablets or dragee cores. Suitable excipients are, in particular, fillers such as sugars, including lactose, sucrose, mannitol, or sorbitol; cellulose preparations such as, for example, maize starch, wheat starch, rice starch, potato starch, gelatin, gum tragacanth, methyl cellulose, hydroxypropylmethyl-cellulose, sodium carboxymethylcellulose, and/or polyvinylpyrrolidone (PVP). If desired, disintegrating agents may be added, such as the cross-linked polyvinyl pyrrolidone, agar, or alginic acid or a salt thereof such as sodium alginate. Dragee cores are provided with suitable coatings. For this purpose, concentrated sugar solutions may be used, which may optionally contain gum arabic. tale, polyvinyl pyrrolidone, carbopol gel, polyethylene glycol, and/or titanium dioxide, lacquer solutions, and suitable organic solvents or solvent mixtures. Dyestuffs or pigments may be added to the tablets or dragee coatings for identification or to characterize different combinations of active compound doses.

Pharmaceutical preparations which can be used orally include push-fit capsules made of gelatin, as well as soft, sealed capsules made of gelatin and a plasticizer, such as glycerol or sorbitol. The push-fit capsules can contain the active ingredients in admixture with filler such as lactose, binders such as starches, and/or lubricants such as talc or magnesium stearate and, optionally, stabilizers. In soft capsules, the active compounds may be dissolved or suspended in suitable liquids, such as fatty oils, liquid paraffin, or liquid polyethylene glycols. In addition,

stabilizers may be added. All formulations for oral administration should be in dosages suitable for such administration. For buccal administration, the compositions may take the form of tablets or lozenges formulated in conventional manner.

For administration by inhalation, the compounds for use according to the present invention are conveniently delivered in the form of an aerosol spray presentation from pressurized packs or a nebuliser, with the use of a suitable propellant, e.g., dichlorodifluoromethane, trichlorofluoromethane, dichlorotetrafluoroethane, carbon dioxide or other suitable gas. In the case of a pressurized aerosol the dosage unit may be determined by providing a valve to deliver a metered amount. Capsules and cartridges of, e.g., gelatin for use in an inhaler or insufflator may be formulated containing a powder mix of the compound and a suitable powder base such as lactose or starch. The compounds may be formulated for parenteral administration by injection, e.g., by bolus injection or continuous infusion. Formulations for injection may be presented in unit dosage form, e.g., in ampules or in multi-dose containers, with an added preservative. The compositions may take such forms as suspensions, solutions or emulsions in oily or aqueous vehicles, and may contain formulatory agents such as suspending, stabilizing and/or dispersing agents.

Pharmaceutical formulations for parenteral administration include aqueous solutions of the active compounds in water-soluble form. Additionally, suspensions of the active compounds may be prepared as appropriate oily injection suspensions. Suitable lipophilic solvents or vehicles include fatty oils such as sesame oil, or synthetic fatty acid esters, such as ethyl oleate or triglycerides, or liposomes. Aqueous injection suspensions may contain substances which increase the viscosity of the suspension, such as sodium carboxymethyl cellulose, sorbitol, or dextran. Optionally, the suspension may also contain suitable stabilizers or agents which increase the solubility of the compounds to allow for the preparation of highly concentrated solutions. Alternatively, the active ingredient may be in powder form for constitution with a suitable vehicle, e.g., sterile pyrogen-free water, before use.

The compounds may also be formulated in rectal compositions such as suppositories or retention enemas, e.g., containing conventional suppository bases such as cocoa butter or other glycerides. In addition to the formulations described previously, the compounds may also be formulated as a depot preparation. Such long acting formulations may be administered by implantation (for example subcutaneously or intramuscularly) or by intramuscular injection. Thus, for example, the compounds may be formulated with suitable polymeric or hydrophobic materials (for example as an emulsion in an acceptable oil) or ion exchange resins, or as sparingly soluble derivatives, for example, as a sparingly soluble salt.

A pharmaceutical carrier for the hydrophobic compounds of the invention is a co-solvent system comprising benzyl alcohol, a nonpolar surfactant, a water-miscible organic polymer, and an aqueous phase. The co-solvent system may be the VPD co-solvent system. VPD is a solution of 3% w/v benzyl alcohol, 8% w/v of the nonpolar surfactant polysorbate 80, and 65% w/v polyethylene glycol 300, made up to volume in absolute ethanol. The VPD co-solvent system (VPD:5W) consists of VPD diluted 1:1 with a 5% dextrose in water solution. This co-solvent system dissolves hydrophobic compounds well, and itself produces low toxicity upon systemic administration. Naturally, the proportions of a co-solvent system may be varied considerably without destroying its solubility and toxicity characteristics. Furthermore, the identity of the co-solvent components may be varied; for example, other low-toxicity nonpolar surfactants may be used instead of polysorbate 80; the fraction size of polyethylene glycol may be varied; other biocompatible polymers may replace polyethylene glycol, e.g. polyvinyl pyrrolidone; and other sugars or polysaccharides may substitute for dextrose. Alternatively, other delivery systems for hydrophobic pharmaceutical compounds may be employed. Liposomes and emulsions are well known examples of delivery vehicles or carriers for hydrophobic drugs. Certain organic solvents such as dimethylsulfoxide also may be employed, although usually at the cost of greater toxicity. Additionally, the compounds may be delivered using a sustained-release system, such as semipermeable matrices of solid hydrophobic polymers containing the therapeutic agent. Various types of sustained-release materials have been established and are well known by those skilled in the art. Sustained-release capsules may, depending on their chemical nature, release the compounds for a few weeks up to over 100 days. Depending on the chemical nature and the biological stability of the therapeutic reagent, additional strategies for protein or other active ingredient stabilization may be employed.

The pharmaceutical compositions also may comprise suitable solid or gel phase carriers or excipients. Examples of such carriers or excipients include but are not limited to calcium carbonate, calcium phosphate, various sugars, starches, cellulose derivatives, gelatin, and polymers such as polyethylene glycols. Many of the active ingredients of the invention may be provided as salts with pharmaceutically compatible counter ions. Such pharmaceutically acceptable base addition salts are those salts which retain the biological effectiveness and properties of the free acids and which are obtained by reaction with inorganic or organic bases such as sodium hydroxide, magnesium hydroxide, ammonia, trialkylamine, dialkylamine, monoalkylamine, dibasic amino acids, sodium acetate, potassium benzoate, triethanol amine and the like.

The pharmaceutical composition of the invention may be in the form of a complex of the protein(s) or other active ingredient(s) of present invention along with protein or peptide

antigens. The protein and/or peptide antigen will deliver a stimulatory signal to both B and T lymphocytes. B lymphocytes will respond to antigen through their surface immunoglobulin receptor. T lymphocytes will respond to antigen through the T cell receptor (TCR) following presentation of the antigen by MHC proteins. MHC and structurally related proteins including those encoded by class I and class II MHC genes on host cells will serve to present the peptide antigen(s) to T lymphocytes. The antigen components could also be supplied as purified MHC-peptide complexes alone or with co-stimulatory molecules that can directly signal T cells. Alternatively antibodies able to bind surface immunoglobulin and other molecules on B cells as well as antibodies able to bind the TCR and other molecules on T cells can be combined with the pharmaceutical composition of the invention.

The pharmaceutical composition of the invention may be in the form of a liposome in which protein of the present invention is combined, in addition to other pharmaceutically acceptable carriers, with amphipathic agents such as lipids which exist in aggregated form as micelles, insoluble monolayers, liquid crystals, or lamellar layers in aqueous solution. Suitable lipids for liposomal formulation include, without limitation, monoglycerides, diglycerides, sulfatides, lysolecithins, phospholipids, saponin, bile acids, and the like. Preparation of such liposomal formulations is within the level of skill in the art, as disclosed, for example, in U.S. Patent Nos. 4,235,871; 4,501,728; 4,837,028; and 4,737,323, all of which are incorporated herein by reference.

The amount of protein or other active ingredient of the present invention in the pharmaceutical composition of the present invention will depend upon the nature and severity of the condition being treated, and on the nature of prior treatments which the patient has undergone. Ultimately, the attending physician will decide the amount of protein or other active ingredient of the present invention with which to treat each individual patient. Initially, the attending physician will administer low doses of protein or other active ingredient of the present invention and observe the patient's response. Larger doses of protein or other active ingredient of the present invention may be administered until the optimal therapeutic effect is obtained for the patient, and at that point the dosage is not increased further. It is contemplated that the various pharmaceutical compositions used to practice the method of the present invention should contain about 0.01 ug to about 100 mg (preferably about 0.1 µg to about 10 mg, more preferably about 0.1 µg to about 1 mg) of protein or other active ingredient of the present invention per kg body weight. For compositions of the present invention which are useful for bone, cartilage, tendon or ligament regeneration, the therapeutic method includes administering the composition topically, systematically, or locally as an implant or device. When administered, the therapeutic composition for use in this invention is, of course, in a pyrogen-free, physiologically acceptable

form. Further, the composition may desirably be encapsulated or injected in a viscous form for delivery to the site of bone, cartilage or tissue damage. Topical administration may be suitable for wound healing and tissue repair. Therapeutically useful agents other than a protein or other active ingredient of the invention which may also optionally be included in the composition as described above, may alternatively or additionally, be administered simultaneously or sequentially with the composition in the methods of the invention. Preferably for bone and/or cartilage formation, the composition would include a matrix capable of delivering the protein-containing or other active ingredient-containing composition to the site of bone and/or cartilage damage, providing a structure for the developing bone and cartilage and optimally capable of being resorbed into the body. Such matrices may be formed of materials presently in use for other implanted medical applications.

The choice of matrix material is based on biocompatibility, biodegradability, mechanical properties, cosmetic appearance and interface properties. The particular application of the compositions will define the appropriate formulation. Potential matrices for the compositions may be biodegradable and chemically defined calcium sulfate, tricalcium phosphate. hydroxyapatite, polylactic acid, polyglycolic acid and polyanhydrides. Other potential materials are biodegradable and biologically well-defined, such as bone or dermal collagen. Further matrices are comprised of pure proteins or extracellular matrix components. Other potential matrices are nonbiodegradable and chemically defined, such as sintered hydroxyapatite, bioglass, aluminates, or other ceramics. Matrices may be comprised of combinations of any of the above mentioned types of material, such as polylactic acid and hydroxyapatite or collagen and tricalcium phosphate. The bioceramics may be altered in composition, such as in calcium-aluminate-phosphate and processing to alter pore size, particle size, particle shape, and biodegradability. Presently preferred is a 50:50 (mole weight) copolymer of lactic acid and glycolic acid in the form of porous particles having diameters ranging from 150 to 800 microns. In some applications, it will be useful to utilize a sequestering agent, such as carboxymethyl cellulose or autologous blood clot, to prevent the protein compositions from disassociating from the matrix.

A preferred family of sequestering agents is cellulosic materials such as alkylcelluloses (including hydroxyalkylcelluloses), including methylcellulose, ethylcellulose, hydroxyethylcellulose, hydroxypropyl-methylcellulose, and carboxymethylcellulose, the most preferred being cationic salts of carboxymethylcellulose (CMC). Other preferred sequestering agents include hyaluronic acid, sodium alginate, poly(ethylene glycol), polyoxyethylene oxide, carboxyvinyl polymer and poly(vinyl alcohol). The amount of sequestering agent useful herein is 0.5-20 wt %, preferably 1-10 wt % based on

total formulation weight, which represents the amount necessary to prevent desorption of the protein from the polymer matrix and to provide appropriate handling of the composition, yet not so much that the progenitor cells are prevented from infiltrating the matrix, thereby providing the protein the opportunity to assist the osteogenic activity of the progenitor cells. In further compositions, proteins or other active ingredients of the invention may be combined with other agents beneficial to the treatment of the bone and/or cartilage defect, wound, or tissue in question. These agents include various growth factors such as epidermal growth factor (EGF), platelet derived growth factor (PDGF), transforming growth factors (TGF- α and TGF- β), and insulin-like growth factor (IGF).

The therapeutic compositions are also presently valuable for veterinary applications. Particularly domestic animals and thoroughbred horses, in addition to humans, are desired patients for such treatment with proteins or other active ingredients of the present invention. The dosage regimen of a protein-containing pharmaceutical composition to be used in tissue regeneration will be determined by the attending physician considering various factors which modify the action of the proteins, e.g., amount of tissue weight desired to be formed, the site of damage, the condition of the damaged tissue, the size of a wound, type of damaged tissue (e.g., bone), the patient's age, sex, and diet, the severity of any infection, time of administration and other clinical factors. The dosage may vary with the type of matrix used in the reconstitution and with inclusion of other proteins in the pharmaceutical composition. For example, the addition of other known growth factors, such as IGF I (insulin like growth factor I), to the final composition, may also effect the dosage. Progress can be monitored by periodic assessment of tissue/bone growth and/or repair, for example, X-rays, histomorphometric determinations and tetracycline labeling.

Polynucleotides of the present invention can also be used for gene therapy. Such polynucleotides can be introduced either in vivo or ex vivo into cells for expression in a mammalian subject. Polynucleotides of the invention may also be administered by other known methods for introduction of nucleic acid into a cell or organism (including, without limitation, in the form of viral vectors or naked DNA). Cells may also be cultured ex vivo in the presence of proteins of the present invention in order to proliferate or to produce a desired effect on or activity in such cells. Treated cells can then be introduced in vivo for therapeutic purposes.

4.12.3 EFFECTIVE DOSAGE

Pharmaceutical compositions suitable for use in the present invention include compositions wherein the active ingredients are contained in an effective amount to achieve its intended purpose. More specifically, a therapeutically effective amount means an amount

effective to prevent development of or to alleviate the existing symptoms of the subject being treated. Determination of the effective amount is well within the capability of those skilled in the art, especially in light of the detailed disclosure provided herein. For any compound used in the method of the invention, the therapeutically effective dose can be estimated initially from appropriate in vitro assays. For example, a dose can be formulated in animal models to achieve a circulating concentration range that can be used to more accurately determine useful doses in humans. For example, a dose can be formulated in animal models to achieve a circulating concentration range that includes the IC50 as determined in cell culture (i.e., the concentration of the test compound which achieves a half-maximal inhibition of the protein's biological activity). Such information can be used to more accurately determine useful doses in humans.

A therapeutically effective dose refers to that amount of the compound that results in amelioration of symptoms or a prolongation of survival in a patient. Toxicity and therapeutic efficacy of such compounds can be determined by standard pharmaceutical procedures in cell cultures or experimental animals, e.g., for determining the LD50 (the dose lethal to 50% of the population) and the ED₅₀ (the dose therapeutically effective in 50% of the population). The dose ratio between toxic and therapeutic effects is the therapeutic index and it can be expressed as the ratio between LD₅₀ and ED₅₀. Compounds which exhibit high therapeutic indices are preferred. The data obtained from these cell culture assays and animal studies can be used in formulating a range of dosage for use in human. The dosage of such compounds lies preferably within a range of circulating concentrations that include the ED50 with little or no toxicity. The dosage may vary within this range depending upon the dosage form employed and the route of administration utilized. The exact formulation, route of administration and dosage can be chosen by the individual physician in view of the patient's condition. See, e.g., Fingl et al., 1975, in "The Pharmacological Basis of Therapeutics", Ch. 1 p.1. Dosage amount and interval may be adjusted individually to provide plasma levels of the active mojety which are sufficient to maintain the desired effects, or minimal effective concentration (MEC). The MEC will vary for each compound but can be estimated from in vitro data. Dosages necessary to achieve the MEC will depend on individual characteristics and route of administration. However, HPLC assays or bioassays can be used to determine plasma concentrations.

Dosage intervals can also be determined using MEC value. Compounds should be administered using a regimen which maintains plasma levels above the MEC for 10-90% of the time, preferably between 30-90% and most preferably between 50-90%. In cases of local administration or selective uptake, the effective local concentration of the drug may not be related to plasma concentration.

An exemplary dosage regimen for polypeptides or other compositions of the invention will be in the range of about $0.01~\mu g/kg$ to 100~mg/kg of body weight daily, with the preferred dose being about $0.1~\mu g/kg$ to 25~mg/kg of patient body weight daily, varying in adults and children. Dosing may be once daily, or equivalent doses may be delivered at longer or shorter intervals.

The amount of composition administered will, of course, be dependent on the subject being treated, on the subject's age and weight, the severity of the affliction, the manner of administration and the judgment of the prescribing physician.

4.12.4 PACKAGING

The compositions may, if desired, be presented in a pack or dispenser device which may contain one or more unit dosage forms containing the active ingredient. The pack may, for example, comprise metal or plastic foil, such as a blister pack. The pack or dispenser device may be accompanied by instructions for administration. Compositions comprising a compound of the invention formulated in a compatible pharmaceutical carrier may also be prepared, placed in an appropriate container, and labeled for treatment of an indicated condition.

4.13 ANTIBODIES

Also included in the invention are antibodies to proteins, or fragments of proteins of the invention. The term "antibody" as used herein refers to immunoglobulin molecules and immunologically active portions of immunoglobulin (Ig) molecules, i.e., molecules that contain an antigen binding site that specifically binds (immunoreacts with) an antigen. Such antibodies include, but are not limited to, polyclonal, monoclonal, chimeric, single chain, F_{ab} , F_{ab} , and $F_{(ab)2}$ fragments, and an F_{ab} expression library. In general, an antibody molecule obtained from humans relates to any of the classes IgG, IgM, IgA, IgE and IgD, which differ from one another by the nature of the heavy chain present in the molecule. Certain classes have subclasses as well, such as IgG1, IgG2, and others. Furthermore, in humans, the light chain may be a kappa chain or a lambda chain. Reference herein to antibodies includes a reference to all such classes, subclasses and types of human antibody species.

An isolated related protein of the invention may be intended to serve as an antigen, or a portion or fragment thereof, and additionally can be used as an immunogen to generate antibodies that immunospecifically bind the antigen, using standard techniques for polyclonal and monoclonal antibody preparation. The full-length protein can be used or, alternatively, the invention provides antigenic peptide fragments of the antigen for use as immunogens. An antigenic peptide fragment comprises at least 6 amino acid residues of the amino acid sequence

of the full length protein, such as the amino acid sequences shown in SEQ ID NO: 445-888, and encompasses an epitope thereof such that an antibody raised against the peptide forms a specific immune complex with the full length protein or with any fragment that contains the epitope. Preferably, the antigenic peptide comprises at least 10 amino acid residues, or at least 15 amino acid residues, or at least 20 amino acid residues, or at least 30 amino acid residues. Preferred epitopes encompassed by the antigenic peptide are regions of the protein that are located on its surface; commonly these are hydrophilic regions.

In certain embodiments of the invention, at least one epitope encompassed by the antigenic peptide is a region of -related protein that is located on the surface of the protein, e.g., a hydrophilic region. A hydrophobicity analysis of the human related protein sequence will indicate which regions of a related protein are particularly hydrophilic and, therefore, are likely to encode surface residues useful for targeting antibody production. As a means for targeting antibody production, hydropathy plots showing regions of hydrophilicity and hydrophobicity may be generated by any method well known in the art, including, for example, the Kyte Doolittle or the Hopp Woods methods, either with or without Fourier transformation. See, e.g., Hopp and Woods, 1981, Proc. Nat. Acad. Sci. USA 78: 3824-3828; Kyte and Doolittle 1982, J. Mol. Biol. 157: 105-142, each of which is incorporated herein by reference in its entirety. Antibodies that are specific for one or more domains within an antigenic protein, or derivatives, fragments, analogs or homologs thereof, are also provided herein.

A protein of the invention, or a derivative, fragment, analog, homolog or ortholog thereof, may be utilized as an immunogen in the generation of antibodies that immunospecifically bind these protein components.

Various procedures known within the art may be used for the production of polyclonal or monoclonal antibodies directed against a protein of the invention, or against derivatives, fragments, analogs homologs or orthologs thereof (see, for example, Antibodies: A Laboratory Manual, Harlow E, and Lane D, 1988, Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY, incorporated herein by reference). Some of these antibodies are discussed below.

4.13.1 POLYCLONAL ANTIBODIES

For the production of polyclonal antibodies, various suitable host animals (e.g., rabbit, goat, mouse or other mammal) may be immunized by one or more injections with the native protein, a synthetic variant thereof, or a derivative of the foregoing. An appropriate immunogenic preparation can contain, for example, the naturally occurring immunogenic protein, a chemically synthesized polypeptide representing the immunogenic protein, or a recombinantly expressed immunogenic protein. Furthermore, the protein may be conjugated to

a second protein known to be immunogenic in the mammal being immunized. Examples of such immunogenic proteins include but are not limited to keyhole limpet hemocyanin, serum albumin, bovine thyroglobulin, and soybean trypsin inhibitor. The preparation can further include an adjuvant. Various adjuvants used to increase the immunological response include, but are not limited to, Freund's (complete and incomplete), mineral gels (e.g., aluminum hydroxide), surface active substances (e.g., lysolecithin, pluronic polyols, polyanions, peptides, oil emulsions, dinitrophenol, etc.), adjuvants usable in humans such as Bacille Calmette-Guerin and Corynebacterium parvum, or similar immunostimulatory agents. Additional examples of adjuvants which can be employed include MPL-TDM adjuvant (monophosphoryl Lipid A, synthetic trehalose dicorynomycolate).

The polyclonal antibody molecules directed against the immunogenic protein can be isolated from the mammal (e.g., from the blood) and further purified by well known techniques, such as affinity chromatography using protein A or protein G, which provide primarily the IgG fraction of immune serum. Subsequently, or alternatively, the specific antigen which is the target of the immunoglobulin sought, or an epitope thereof, may be immobilized on a column to purify the immune specific antibody by immunoaffinity chromatography. Purification of immunoglobulins is discussed, for example, by D. Wilkinson (The Scientist, published by The Scientist, Inc., Philadelphia PA, Vol. 14, No. 8 (April 17, 2000), pp. 25-28).

4.13.2 MONOCLONAL ANTIBODIES

The term "monoclonal antibody" (MAb) or "monoclonal antibody composition", as used herein, refers to a population of antibody molecules that contain only one molecular species of antibody molecule consisting of a unique light chain gene product and a unique heavy chain gene product. In particular, the complementarity determining regions (CDRs) of the monoclonal antibody are identical in all the molecules of the population. MAbs thus contain an antigen binding site capable of immunoreacting with a particular epitope of the antigen characterized by a unique binding affinity for it.

Monoclonal antibodies can be prepared using hybridoma methods, such as those described by Kohler and Milstein, Nature, 256:495 (1975). In a hybridoma method, a mouse, hamster, or other appropriate host animal, is typically immunized with an immunizing agent to elicit lymphocytes that produce or are capable of producing antibodies that will specifically bind to the immunizing agent. Alternatively, the lymphocytes can be immunized in vitro.

The immunizing agent will typically include the protein antigen, a fragment thereof or a fusion protein thereof. Generally, either peripheral blood lymphocytes are used if cells of human origin are desired, or spleen cells or lymph node cells are used if non-human mammalian sources are

desired. The lymphocytes are then fused with an immortalized cell line using a suitable fusing agent, such as polyethylene glycol, to form a hybridoma cell (Goding, Monoclonal Antibodies: Principles and Practice, Academic Press, (1986) pp. 59-103). Immortalized cell lines are usually transformed mammalian cells, particularly myeloma cells of rodent, bovine and human origin. Usually, rat or mouse myeloma cell lines are employed. The hybridoma cells can be cultured in a suitable culture medium that preferably contains one or more substances that inhibit the growth or survival of the unfused, immortalized cells. For example, if the parental cells lack the enzyme hypoxanthine guanine phosphoribosyl transferase (HGPRT or HPRT), the culture medium for the hybridomas typically will include hypoxanthine, aminopterin, and thymidine ("HAT medium"), which substances prevent the growth of HGPRT-deficient cells.

Preferred immortalized cell lines are those that fuse efficiently, support stable high level expression of antibody by the selected antibody-producing cells, and are sensitive to a medium such as HAT medium. More preferred immortalized cell lines are murine myeloma lines, which can be obtained, for instance, from the Salk Institute Cell Distribution Center, San Diego, California and the American Type Culture Collection, Manassas, Virginia. Human myeloma and mouse-human heteromyeloma cell lines also have been described for the production of human monoclonal antibodies (Kozbor, J. Immunol., 133:3001 (1984); Brodeur et al., Monoclonal Antibody Production Techniques and Applications, Marcel Dekker, Inc., New York, (1987) pp. 51-63).

The culture medium in which the hybridoma cells are cultured can then be assayed for the presence of monoclonal antibodies directed against the antigen. Preferably, the binding specificity of monoclonal antibodies produced by the hybridoma cells is determined by immunoprecipitation or by an in vitro binding assay, such as radioimmunoassay (RIA) or enzyme-linked immunoabsorbent assay (ELISA). Such techniques and assays are known in the art. The binding affinity of the monoclonal antibody can, for example, be determined by the Scatchard analysis of Munson and Pollard, Anal. Biochem., 107:220 (1980). Preferably, antibodies having a high degree of specificity and a high binding affinity for the target antigen are isolated.

After the desired hybridoma cells are identified, the clones can be subcloned by limiting dilution procedures and grown by standard methods. Suitable culture inedia for this purpose include, for example, Dulbecco's Modified Eagle's Medium and RPMI-1640 medium.

Alternatively, the hybridoma cells can be grown in vivo as ascites in a mammal.

The monoclonal antibodies secreted by the subclones can be isolated or purified from the culture medium or ascites fluid by conventional immunoglobulin purification procedures such as, for

example, protein A-Sepharose, hydroxylapatite chromatography, gel electrophoresis, dialysis, or affinity chromatography.

The monoclonal antibodies can also be made by recombinant DNA methods, such as those described in U.S. Patent No. 4,816,567. DNA encoding the monoclonal antibodies of the invention can be readily isolated and sequenced using conventional procedures (e.g., by using oligonucleotide probes that are capable of binding specifically to genes encoding the heavy and light chains of murine antibodies). The hybridoma cells of the invention serve as a preferred source of such DNA. Once isolated, the DNA can be placed into expression vectors, which are then transfected into host cells such as simian COS cells. Chinese hamster ovary (CHO) cells, or myeloma cells that do not otherwise produce immunoglobulin protein, to obtain the synthesis of monoclonal antibodies in the recombinant host cells. The DNA also can be modified, for example, by substituting the coding sequence for human heavy and light chain constant domains in place of the homologous murine sequences (U.S. Patent No. 4,816,567; Morrison, Nature 368, 812-13 (1994)) or by covalently joining to the immunoglobulin coding sequence all or part of the coding sequence for a non-immunoglobulin polypeptide. Such a non-immunoglobulin polypeptide can be substituted for the constant domains of an antibody of the invention, or can be substituted for the variable domains of one antigen-combining site of an antibody of the invention to create a chimeric bivalent antibody.

4.13.3 HUMANIZED ANTIBODIES

The antibodies directed against the protein antigens of the invention can further comprise humanized antibodies or human antibodies. These antibodies are suitable for administration to humans without engendering an immune response by the human against the administered immunoglobulin. Humanized forms of antibodies are chimeric immunoglobulins, immunoglobulin chains or fragments thereof (such as Fv, Fab, Fab', F(ab')2 or other antigenbinding subsequences of antibodies) that are principally comprised of the sequence of a human immunoglobulin, and contain minimal sequence derived from a non-human immunoglobulin. Humanization can be performed following the method of Winter and co-workers (Jones et al., Nature, 321:522-525 (1986); Riechmann et al., Nature, 332:323-327 (1988); Verhoeyen et al., Science, 239:1534-1536 (1988)), by substituting rodents CDRs or CDR sequences for the corresponding sequences of a human antibody. (See also U.S. Patent No. 5,225,539.) In some instances, Fv framework residues of the human immunoglobulin are replaced by corresponding non-human residues. Humanized antibodies can also comprise residues which are found neither in the recipient antibody nor in the imported CDR or framework sequences. In general, the humanized antibody will comprise substantially all of at least one, and typically two, variable

domains, in which all or substantially all of the CDR regions correspond to those of a non-human immunoglobulin and all or substantially all of the framework regions are those of a human immunoglobulin consensus sequence. The humanized antibody optimally also will comprise at least a portion of an immunoglobulin constant region (Fc), typically that of a human immunoglobulin (Jones et al., 1986; Riechmann et al., 1988; and Presta, <u>Curr. Op. Struct. Biol.</u>, 2:593-596 (1992)).

4.13.4 HUMAN ANTIBODIES

Fully human antibodies relate to antibody molecules in which essentially the entire sequences of both the light chain and the heavy chain, including the CDRs, arise from human genes. Such antibodies are termed "human antibodies", or "fully human antibodies" herein. Human monoclonal antibodies can be prepared by the trioma technique; the human B-cell hybridoma technique (see Kozbor, et al., 1983 Immunol Today 4: 72) and the EBV hybridoma technique to produce human monoclonal antibodies (see Cole, et al., 1985 In: MONOCLONAL ANTIBODIES AND CANCER THERAPY, Alan R. Liss, Inc., pp. 77-96). Human monoclonal antibodies may be utilized in the practice of the present invention and may be produced by using human hybridomas (see Cote, et al., 1983. Proc Natl Acad Sci USA 80: 2026-2030) or by transforming human B-cells with Epstein Barr Virus in vitro (see Cole, et al., 1985 In: MONOCLONAL ANTIBODIES AND CANCER THERAPY, Alan R. Liss, Inc., pp. 77-96).

In addition, human antibodies can also be produced using additional techniques, including phage display libraries (Hoogenboom and Winter, J. Mol. Biol., 227:381 (1991); Marks et al., J. Mol. Biol., 222:581 (1991)). Similarly, human antibodies can be made by introducing human immunoglobulin loci into transgenic animals, e.g., mice in which the endogenous immunoglobulin genes have been partially or completely inactivated. Upon challenge, human antibody production is observed, which closely resembles that seen in humans in all respects, including gene rearrangement, assembly, and antibody repertoire. This approach is described, for example, in U.S. Patent Nos. 5,545,807; 5,545,806; 5,569,825; 5,625,126; 5,633,425; 5,661,016, and in Marks et al. (Bio/Technology 10, 779-783 (1992)); Lonberg et al. (Nature 368 856-859 (1994)); Morrison (Nature 368, 812-13 (1994)); Fishwild et al., (Nature Biotechnology 14, 845-51 (1996)); Neuberger (Nature Biotechnology 14, 826 (1996)); and Lonberg and Huszar (Intern. Rev. Immunol, 13 65-93 (1995)).

Human antibodies may additionally be produced using transgenic nonhuman animals which are modified so as to produce fully human antibodies rather than the animal's endogenous antibodies in response to challenge by an antigen. (See PCT publication WO94/02602). The endogenous genes encoding the heavy and light immunoglobulin chains in the nonhuman host

have been incapacitated, and active loci encoding human heavy and light chain immunoglobulins are inserted into the host's genome. The human genes are incorporated, for example, using yeast artificial chromosomes containing the requisite human DNA segments. An animal which provides all the desired modifications is then obtained as progeny by crossbreeding intermediate transgenic animals containing fewer than the full complement of the modifications. The preferred embodiment of such a nonhuman animal is a mouse, and is termed the Xenomouse™ as disclosed in PCT publications WO 96/33735 and WO 96/34096. This animal produces B cells which secrete fully human immunoglobulins. The antibodies can be obtained directly from the animal after immunization with an immunogen of interest, as, for example, a preparation of a polyclonal antibody, or alternatively from immortalized B cells derived from the animal, such as hybridomas producing monoclonal antibodies. Additionally, the genes encoding the immunoglobulins with human variable regions can be recovered and expressed to obtain the antibodies directly, or can be further modified to obtain analogs of antibodies such as, for example, sincle chain Fy molecules.

An example of a method of producing a nonhuman host, exemplified as a mouse, lacking expression of an endogenous immunoglobulin heavy chain is disclosed in U.S. Patent No. 5,939,598. It can be obtained by a method including deleting the J segment genes from at least one endogenous heavy chain locus in an embryonic stem cell to prevent rearrangement of the locus and to prevent formation of a transcript of a rearranged immunoglobulin heavy chain locus, the deletion being effected by a targeting vector containing a gene encoding a selectable marker; and producing from the embryonic stem cell a transgenic mouse whose somatic and germ cells contain the gene encoding the selectable marker.

A method for producing an antibody of interest, such as a human antibody, is disclosed in U.S. Patent No. 5,916,771. It includes introducing an expression vector that contains a nucleotide sequence encoding a heavy chain into one mammalian host cell in culture, introducing an expression vector containing a nucleotide sequence encoding a light chain into another mammalian host cell, and fusing the two cells to form a hybrid cell. The hybrid cell expresses an antibody containing the heavy chain and the light chain.

In a further improvement on this procedure, a method for identifying a clinically relevant epitope on an immunogen, and a correlative method for selecting an antibody that binds immunospecifically to the relevant epitope with high affinity, are disclosed in PCT publication WO 99/53049.

4.13.5 For FRAGMENTS AND SINGLE CHAIN ANTIBODIES

According to the invention, techniques can be adapted for the production of single-chain antibodies specific to an antigenic protein of the invention (see e.g., U.S. Patent No. 4,946,778). In addition, methods can be adapted for the construction of F_{ab} expression libraries (see e.g., Huse, et al., 1989 Science 246: 1275-1281) to allow rapid and effective identification of monoclonal F_{ab} fragments with the desired specificity for a protein or derivatives, fragments, analogs or homologs thereof. Antibody fragments that contain the idiotypes to a protein antigen may be produced by techniques known in the art including, but not limited to: (i) an $F_{(ab)/2}$ fragment produced by pepsin digestion of an antibody molecule; (ii) an F_{ab} fragment generated by reducing the disulfide bridges of an $F_{(ab)/2}$ fragment; (iii) an F_{ab} fragment generated by the treatment of the antibody molecule with papain and a reducing agent and (iv) F_{v} fragments.

4.13.6 BISPECIFIC ANTIBODIES

Bispecific antibodies are monoclonal, preferably human or humanized, antibodies that have binding specificities for at least two different antigens. In the present case, one of the binding specificities is for an antigenic protein of the invention. The second binding target is any other antigen, and advantageously is a cell-surface protein or receptor or receptor subunit.

Methods for making bispecific antibodies are known in the art. Traditionally, the recombinant production of bispecific antibodies is based on the co-expression of two immunoglobulin heavy-chain/light-chain pairs, where the two heavy chains have different specificities (Milstein and Cuello, Nature, 305:537-539 (1983)). Because of the random assortment of immunoglobulin heavy and light chains, these hybridomas (quadromas) produce a potential mixture of ten different antibody molecules, of which only one has the correct bispecific structure. The purification of the correct molecule is usually accomplished by affinity chromatography steps. Similar procedures are disclosed in WO 93/08829, published 13 May 1993, and in Traunecker et al., 1991 EMBO J., 10:3655-3659.

Antibody variable domains with the desired binding specificities (antibody-antigen combining sites) can be fused to immunoglobulin constant domain sequences. The fusion preferably is with an immunoglobulin heavy-chain constant domain, comprising at least part of the hinge, CH2, and CH3 regions. It is preferred to have the first heavy-chain constant region (CH1) containing the site necessary for light-chain binding present in at least one of the fusions. DNAs encoding the immunoglobulin heavy-chain fusions and, if desired, the immunoglobulin light chain, are inserted into separate expression vectors, and are co-transfected into a suitable host organism. For further details of generating bispecific antibodies see, for example, Suresh et al., Methods in Enzymology, 121:210 (1986).

According to another approach described in WO 96/27011, the interface between a pair of antibody molecules can be engineered to maximize the percentage of heterodimers which are recovered from recombinant cell culture. The preferred interface comprises at least a part of the CH3 region of an antibody constant domain. In this method, one or more small amino acid side chains from the interface of the first antibody molecule are replaced with larger side chains (e.g. tyrosine or tryptophan). Compensatory "cavities" of identical or similar size to the large side chain(s) are created on the interface of the second antibody molecule by replacing large amino acid side chains with smaller ones (e.g. alanine or threonine). This provides a mechanism for increasing the yield of the heterodimer over other unwanted end-products such as homodimers.

Bispecific antibodies can be prepared as full length antibodies or antibody fragments (e.g. F(ab')₂ bispecific antibodies). Techniques for generating bispecific antibodies from antibody fragments have been described in the literature. For example, bispecific antibodies can be prepared using chemical linkage. Brennan et al., Science 229:81 (1985) describe a procedure wherein intact antibodies are proteolytically cleaved to generate F(ab')₂ fragments. These fragments are reduced in the presence of the dithiol complexing agent sodium arsenite to stabilize vicinal dithiols and prevent intermolecular disulfide formation. The Fab' fragments generated are then converted to thionitrobenzoate (TNB) derivatives. One of the Fab'-TNB derivatives is then reconverted to the Fab'-thiol by reduction with mercaptoethylamine and is mixed with an equimolar amount of the other Fab'-TNB derivative to form the bispecific antibodies produced can be used as agents for the selective immobilization of enzymes.

Additionally, Fab' fragments can be directly recovered from E. coli and chemically coupled to form bispecific antibodies. Shalaby et al., J. Exp. Med. 175:217-225 (1992) describe the production of a fully humanized bispecific antibody F(ab')₂ molecule. Each Fab' fragment was separately secreted from E. coli and subjected to directed chemical coupling in vitro to form the bispecific antibody. The bispecific antibody thus formed was able to bind to cells overexpressing the ErbB2 receptor and normal human T cells, as well as trigger the lytic activity of human cytotoxic lymphocytes against human breast tumor targets.

Various techniques for making and isolating bispecific antibody fragments directly from recombinant cell culture have also been described. For example, bispecific antibodies have been produced using leucine zippers. Kostelny et al., J. Immunol. 148(5):1547-1553 (1992). The leucine zipper peptides from the Fos and Jun proteins were linked to the Fab' portions of two different antibodies by gene fusion. The antibody homodimers were reduced at the hinge region to form monomers and then re-oxidized to form the antibody heterodimers. This method can also be utilized for the production of antibody homodimers. The "diabody" technology

described by Hollinger et al., <u>Proc. Natl. Acad. Sci. USA</u> 90:6444-6448 (1993) has provided an alternative mechanism for making bispecific antibody fragments. The fragments comprise a heavy-chain variable domain (V_H) connected to a light-chain variable domain (V_L) by a linker which is too short to allow pairing between the two domains on the same chain. Accordingly, the V_H and V_L domains of one fragment are forced to pair with the complementary V_L and V_H domains of another fragment, thereby forming two antigen-binding sites. Another strategy for making bispecific antibody fragments by the use of single-chain Fv (sFv) dimers has also been reported. See, Gruber et al., J. Immunol. 152:5368 (1994).

Antibodies with more than two valencies are contemplated. For example, trispecific antibodies can be prepared. Tutt et al., <u>J. Immunol.</u> 147:60 (1991). Exemplary bispecific antibodies can bind to two different epitopes, at least one of which originates in the protein antigen of the invention. Alternatively, an anti-antigenic arm of an immunoglobulin molecule can be combined with an arm which binds to a triggering molecule a leukocyte such as a T-cell receptor molecule (e.g. CD2, CD3, CD28, or B7), or Fc receptors in the contemplated of the contemplated of the contemplated.

originates in the protein antigen of the invention. Alternatively, an anti-antigenic arm of an immunoglobulin molecule can be combined with an arm which binds to a triggering molecule on a leukocyte such as a T-cell receptor molecule (e.g. CD2, CD3, CD28, or B7), or Fc receptors for IgG (FcyR), such as FcyRI (CD64), FcyRII (CD32) and FcyRIII (CD16) so as to focus cellular defense mechanisms to the cell expressing the particular antigen. Bispecific antibodies can also be used to direct cytotoxic agents to cells which express a particular antigen. These antibodies possess an antigen-binding arm and an arm which binds a cytotoxic agent or a radionuclide chelator, such as EOTUBE, DPTA, DOTA, or TETA. Another bispecific antibody of interest binds the protein antigen described herein and further binds tissue factor (TF).

4.13.7 HETEROCONJUGATE ANTIBODIES

Heteroconjugate antibodies are also within the scope of the present invention.

Heteroconjugate antibodies are composed of two covalently joined antibodies. Such antibodies have, for example, been proposed to target immune system cells to unwanted cells (U.S. Patent No. 4,676,980), and for treatment of HIV infection (WO 91/00360; WO 92/200373; EP 03089). It is contemplated that the antibodies can be prepared in vitro using known methods in synthetic protein chemistry, including those involving crosslinking agents. For example, immunotoxins can be constructed using a disulfide exchange reaction or by forming a thioether bond. Examples of suitable reagents for this purpose include immothiolate and methyl-4-mercaptobutyrimidate and those disclosed, for example, in U.S. Patent No. 4,676,980.

4.13.8 EFFECTOR FUNCTION ENGINEERING

It can be desirable to modify the antibody of the invention with respect to effector function, so as to enhance, e.g., the effectiveness of the antibody in treating cancer. For example, cysteine residue(s) can be introduced into the Fc region, thereby allowing interchain disulfide bond formation in this region. The homodimeric antibody thus generated can have improved internalization capability and/or increased complement-mediated cell killing and antibody-dependent cellular cytotoxicity (ADCC). See Caron et al., J. Exp Med., 176: 1191-1195 (1992) and Shopes, J. Immunol., 148: 2918-2922 (1992). Homodimeric antibodies with enhanced antitumor activity can also be prepared using heterobifunctional cross-linkers as described in Wolff et al. Cancer Research, 53: 2560-2565 (1993). Alternatively, an antibody can be engineered that has dual Fc regions and can thereby have enhanced complement lysis and ADCC capabilities. See Stevenson et al., Anti-Cancer Drug Design, 3: 219-230 (1989).

4.13.9 IMMUNOCONJUGATES

The invention also pertains to immunoconjugates comprising an antibody conjugated to a cytotoxic agent such as a chemotherapeutic agent, toxin (e.g., an enzymatically active toxin of bacterial, fungal, plant, or animal origin, or fragments thereof), or a radioactive isotope (i.e., a radioconjugate).

Chemotherapeutic agents useful in the generation of such immunoconjugates have been described above. Enzymatically active toxins and fragments thereof that can be used include diphtheria A chain, nonbinding active fragments of diphtheria toxin, exotoxin A chain (from Pseudomonas aeruginosa), ricin A chain, abrin A chain, modeccin A chain, alpha-sarcin, Aleurites fordii proteins, dianthin proteins, Phytolaca americana proteins (PAPI, PAPII, and PAP-S), momordica charantia inhibitor, curcin, crotin, sapaonaria officinalis inhibitor, gelonin, mitogellin, restrictocin, phenomycin, enomycin, and the tricothecenes. A variety of radionuclides are available for the production of radioconjugated antibodies. Examples include ²¹²Bi. ¹³¹I. ¹³¹In. ⁹⁰Y, and ¹⁸⁶Re.

Conjugates of the antibody and cytotoxic agent are made using a variety of bifunctional protein-coupling agents such as N-succinimidyl-3-(2-pyridyldithiol) propionate (SPDP), iminothiolane (IT), bifunctional derivatives of imidoesters (such as dimethyl adipimidate HCL), active esters (such as disuccinimidyl suberate), aldehydes (such as glutareldehyde), bis-azido compounds (such as bis (p-azidobenzoyl) hexanediamine), bis-diazonium derivatives (such as bis-(p-diazoniumbenzoyl)-ethylenediamine), diisocyanates (such as tolyene 2,6-diisocyanate), and bis-active fluorine compounds (such as 1,5-difluoro-2,4-dinitrobenzene). For example, a ricin immunotoxin can be prepared as described in Vitetta et al., Science, 238: 1098 (1987). Carbon-14-labeled 1-isothiocyanatobenzyl-3-methyldiethylene triaminepentaacetic acid (MX-DTPA) is an exemplary chelating agent for conjugation of radionucleotide to the antibody. See WO94/11026.

In another embodiment, the antibody can be conjugated to a "receptor" (such as streptavidin) for utilization in tumor pretargeting wherein the antibody-receptor conjugate is administered to the patient, followed by removal of unbound conjugate from the circulation using a clearing agent and then administration of a "ligand" (e.g., avidin) that is in turn conjugated to a cytotoxic agent.

4.14 COMPUTER READABLE SEQUENCES

In one application of this embodiment, a nucleotide sequence of the present invention can be recorded on computer readable media. As used herein, "computer readable media" refers to any medium which can be read and accessed directly by a computer. Such media include, but are not limited to: magnetic storage media, such as floppy discs, hard disc storage medium, and magnetic tape; optical storage media such as CD-ROM; electrical storage media such as RAM and ROM; and hybrids of these categories such as magnetic/optical storage media. A skilled artisan can readily appreciate how any of the presently known computer readable mediums can be used to create a manufacture comprising computer readable medium having recorded thereon a nucleotide sequence of the present invention. As used herein, "recorded" refers to a process for storing information on computer readable medium. A skilled artisan can readily adopt any of the presently known methods for recording information on computer readable medium to generate manufactures comprising the nucleotide sequence information of the present invention.

A variety of data storage structures are available to a skilled artisan for creating a computer readable medium having recorded thereon a nucleotide sequence of the present invention. The choice of the data storage structure will generally be based on the means chosen to access the stored information. In addition, a variety of data processor programs and formats can be used to store the nucleotide sequence information of the present invention on computer readable medium. The sequence information can be represented in a word processing text file, formatted in commercially-available software such as WordPerfect and Microsoft Word, or represented in the form of an ASCII file, stored in a database application, such as DB2, Sybase, Oracle, or the like. A skilled artisan can readily adapt any number of data processor structuring formats (e.g. text file or database) in order to obtain computer readable medium having recorded thereon the nucleotide sequence information of the present invention.

By providing any of the nucleotide sequences SEQ ID NO: 1-444 or a representative fragment thereof; or a nucleotide sequence at least 95% identical to any of the nucleotide sequences of SEQ ID NO: 1-444 in computer readable form, a skilled artisan can routinely access the sequence information for a variety of purposes. Computer software is publicly available which allows a skilled artisan to access sequence information provided in a computer

readable medium. The examples which follow demonstrate how software which implements the BLAST (Altschul et al., J. Mol. Biol. 215:403-410 (1990)) and BLAZE (Brutlag et al., Comp. Chem. 17:203-207 (1993)) search algorithms on a Sybase system is used to identify open reading frames (ORFs) within a nucleic acid sequence. Such ORFs may be protein encoding fragments and may be useful in producing commercially important proteins such as enzymes used in fermentation reactions and in the production of commercially useful metabolites.

As used herein, "a computer-based system" refers to the hardware means, software means, and data storage means used to analyze the nucleotide sequence information of the present invention. The minimum hardware means of the computer-based systems of the present invention comprises a central processing unit (CPU), input means, output means, and data storage means. A skilled artisan can readily appreciate that any one of the currently available computer-based systems are suitable for use in the present invention. As stated above, the computer-based systems of the present invention comprise a data storage means having stored therein a nucleotide sequence of the present invention and the necessary hardware means and software means for supporting and implementing a search means. As used herein, "data storage means" refers to memory which can store nucleotide sequence information of the present invention, or a memory access means which can access manufactures having recorded thereon the nucleotide sequence information of the present invention.

As used herein, "search means" refers to one or more programs which are implemented on the computer-based system to compare a target sequence or target structural motif with the sequence information stored within the data storage means. Search means are used to identify fragments or regions of a known sequence which match a particular target sequence or target motif. A variety of known algorithms are disclosed publicly and a variety of commercially available software for conducting search means are and can be used in the computer-based systems of the present invention. Examples of such software includes, but is not limited to, Smith-Waterman, MacPattern (EMBL), BLASTN and BLASTA (NPOLYPEPTIDEIA). A skilled artisan can readily recognize that any one of the available algorithms or implementing software packages for conducting homology searches can be adapted for use in the present computer-based systems. As used herein, a "target sequence" can be any nucleic acid or amino acid sequence of six or more nucleotides or two or more amino acids. A skilled artisan can readily recognize that the longer a target sequence is, the less likely a target sequence will be present as a random occurrence in the database. The most preferred sequence length of a target sequence is from about 10 to 300 amino acids, more preferably from about 30 to 100 nucleotide residues. However, it is well recognized that searches for commercially important fragments,

such as sequence fragments involved in gene expression and protein processing, may be of shorter length.

As used herein, "a target structural motif," or "target motif," refers to any rationally selected sequence or combination of sequences in which the sequence(s) are chosen based on a three-dimensional configuration which is formed upon the folding of the target motif. There are a variety of target motifs known in the art. Protein target motifs include, but are not limited to, enzyme active sites and signal sequences. Nucleic acid target motifs include, but are not limited to, promoter sequences, hairpin structures and inducible expression elements (protein binding sequences).

4.15 TRIPLE HELIX FORMATION

In addition, the fragments of the present invention, as broadly described, can be used to control gene expression through triple helix formation or antisense DNA or RNA, both of which methods are based on the binding of a polynucleotide sequence to DNA or RNA.

Polynucleotides suitable for use in these methods are preferably 20 to 40 bases in length and are designed to be complementary to a region of the gene involved in transcription (triple helix - see Lee et al., Nucl. Acids Res. 6:3073 (1979); Cooney et al., Science 15241:456 (1988); and Dervan et al., Science 251:1360 (1991)) or to the mRNA itself (antisense - Olmno, J. Neurochem.

56:560 (1991); Oligodeoxynucleotides as Antisense Inhibitors of Gene Expression, CRC Press, Boca Raton, FL (1988)). Triple helix-formation optimally results in a shut-off of RNA ranscription from DNA, while antisense RNA hybridization blocks translation of an mRNA molecule into polypeptide. Both techniques have been demonstrated to be effective in model systems. Information contained in the sequences of the present invention is necessary for the design of an antisense or triple helix oligonucleotide.

4.16 DIAGNOSTIC ASSAYS AND KITS

The present invention further provides methods to identify the presence or expression of one of the ORFs of the present invention, or homolog thereof, in a test sample, using a nucleic acid probe or antibodies of the present invention, optionally conjugated or otherwise associated with a suitable label.

In general, methods for detecting a polynucleotide of the invention can comprise contacting a sample with a compound that binds to and forms a complex with the polynucleotide for a period sufficient to form the complex, and detecting the complex, so that if a complex is detected, a polynucleotide of the invention is detected in the sample. Such methods can also comprise contacting a sample under stringent hybridization conditions with nucleic acid primers

that anneal to a polynucleotide of the invention under such conditions, and amplifying annealed polynucleotides, so that if a polynucleotide is amplified, a polynucleotide of the invention is detected in the sample.

In general, methods for detecting a polypeptide of the invention can comprise contacting a sample with a compound that binds to and forms a complex with the polypeptide for a period sufficient to form the complex, and detecting the complex, so that if a complex is detected, a polypeptide of the invention is detected in the sample.

In detail, such methods comprise incubating a test sample with one or more of the antibodies or one or more of the nucleic acid probes of the present invention and assaying for binding of the nucleic acid probes or antibodies to components within the test sample.

Conditions for incubating a nucleic acid probe or antibody with a test sample vary. Incubation conditions depend on the format employed in the assay, the detection methods employed, and the type and nature of the nucleic acid probe or antibody used in the assay. One skilled in the art will recognize that any one of the commonly available hybridization, amplification or immunological assay formats can readily be adapted to employ the nucleic acid probes or antibodies of the present invention. Examples of such assays can be found in Chard, T., An Introduction to Radioimmunoassay and Related Techniques, Elsevier Science Publishers, Amsterdam, The Netherlands (1986); Bullock, G.R. et al., Techniques in Immunocytochemistry, Academic Press, Orlando, FL Vol. 1 (1982), Vol. 2 (1983), Vol. 3 (1985); Tijssen, P., Practice and Theory of immunoassays: Laboratory Techniques in Biochemistry and Molecular Biology. Elsevier Science Publishers, Amsterdam, The Netherlands (1985). The test samples of the present invention include cells, protein or membrane extracts of cells, or biological fluids such as sputum, blood, serum, plasma, or urine. The test sample used in the above-described method will vary based on the assay format, nature of the detection method and the tissues, cells or extracts used as the sample to be assayed. Methods for preparing protein extracts or membrane extracts of cells are well known in the art and can be readily be adapted in order to obtain a sample which is compatible with the system utilized.

In another embodiment of the present invention, kits are provided which contain the necessary reagents to carry out the assays of the present invention. Specifically, the invention provides a compartment kit to receive, in close confinement, one or more containers which comprises: (a) a first container comprising one of the probes or antibodies of the present invention; and (b) one or more other containers comprising one or more of the following: wash reagents, reagents capable of detecting presence of a bound probe or antibody.

In detail, a compartment kit includes any kit in which reagents are contained in separate containers. Such containers include small glass containers, plastic containers or strips of plastic

or paper. Such containers allows one to efficiently transfer reagents from one compartment to another compartment such that the samples and reagents are not cross-contaminated, and the agents or solutions of each container can be added in a quantitative fashion from one compartment to another. Such containers will include a container which will accept the test sample, a container which contains the antibodies used in the assay, containers which contain wash reagents (such as phosphate buffered saline, Tris-buffers, etc.), and containers which contain the reagents used to detect the bound antibody or probe. Types of detection reagents include labeled nucleic acid probes, labeled secondary antibodies, or in the alternative, if the primary antibody is labeled, the enzymatic, or antibody binding reagents which are capable of reacting with the labeled antibody. One skilled in the art will readily recognize that the disclosed probes and antibodies of the present invention can be readily incorporated into one of the established kit formats which are well known in the art.

4.17 MEDICAL IMAGING

The novel polypeptides and binding partners of the invention are useful in medical imaging of sites expressing the molecules of the invention (e.g., where the polypeptide of the invention is involved in the immune response, for imaging sites of inflammation or infection). See, e.g., Kunkel et al., U.S. Pat. NO. 5,413,778. Such methods involve chemical attachment of a labeling or imaging agent, administration of the labeled polypeptide to a subject in a pharmaceutically acceptable carrier, and imaging the labeled polypeptide in vivo at the target site.

4.18 SCREENING ASSAYS

Using the isolated proteins and polynucleotides of the invention, the present invention further provides methods of obtaining and identifying agents which bind to a polypeptide encoded by an ORF corresponding to any of the nucleotide sequences set forth in SEQ ID NO: 1-444, or bind to a specific domain of the polypeptide encoded by the nucleic acid. In detail, said method comprises the steps of:

- (a) contacting an agent with an isolated protein encoded by an ORF of the present invention, or nucleic acid of the invention; and
- (b) determining whether the agent binds to said protein or said nucleic acid. In general, therefore, such methods for identifying compounds that bind to a polynucleotide of the invention can comprise contacting a compound with a polynucleotide of the invention for a time sufficient to form a polynucleotide/compound complex, and detecting

the complex, so that if a polynucleotide/compound complex is detected, a compound that binds to a polynucleotide of the invention is identified.

Likewise, in general, therefore, such methods for identifying compounds that bind to a polypeptide of the invention can comprise contacting a compound with a polypeptide of the invention for a time sufficient to form a polypeptide/compound complex, and detecting the complex, so that if a polypeptide/compound complex is detected, a compound that binds to a polynucleotide of the invention is identified.

Methods for identifying compounds that bind to a polypeptide of the invention can also comprise contacting a compound with a polypeptide of the invention in a cell for a time sufficient to form a polypeptide/compound complex, wherein the complex drives expression of a receptor gene sequence in the cell, and detecting the complex by detecting reporter gene sequence expression, so that if a polypeptide/compound complex is detected, a compound that binds a polypeptide of the invention is identified.

Compounds identified via such methods can include compounds which modulate the activity of a polypeptide of the invention (that is, increase or decrease its activity, relative to activity observed in the absence of the compound). Alternatively, compounds identified via such methods can include compounds which modulate the expression of a polynucleotide of the invention (that is, increase or decrease expression relative to expression levels observed in the absence of the compound). Compounds, such as compounds identified via the methods of the invention, can be tested using standard assays well known to those of skill in the art for their ability to modulate activity/expression.

The agents screened in the above assay can be, but are not limited to, peptides, carbohydrates, vitamin derivatives, or other pharmaceutical agents. The agents can be selected and screened at random or rationally selected or designed using protein modeling techniques.

For random screening, agents such as peptides, carbohydrates, pharmaceutical agents and the like are selected at random and are assayed for their ability to bind to the protein encoded by the ORF of the present invention. Alternatively, agents may be rationally selected or designed. As used herein, an agent is said to be "rationally selected or designed" when the agent is chosen based on the configuration of the particular protein. For example, one skilled in the art can readily adapt currently available procedures to generate peptides, pharmaceutical agents and the like, capable of binding to a specific peptide sequence, in order to generate rationally designed antipeptide peptides, for example see Hurby et al., Application of Synthetic Peptides: Antisense Peptides," In Synthetic Peptides, A User's Guide, W.H. Freeman, NY (1992), pp. 289-307, and Kaspczak et al., Biochemistry 28:9230-8 (1989), or pharmaceutical agents, or the like.

In addition to the foregoing, one class of agents of the present invention, as broadly described, can be used to control gene expression through binding to one of the ORFs or EMFs of the present invention. As described above, such agents can be randomly screened or rationally designed/selected. Targeting the ORF or EMF allows a skilled artisan to design sequence specific or element specific agents, modulating the expression of either a single ORF or multiple ORFs which rely on the same EMF for expression control. One class of DNA binding agents are agents which contain base residues which hybridize or form a triple helix formation by binding to DNA or RNA. Such agents can be based on the classic phosphodiester, ribonucleic acid backbone, or can be a variety of sulfhydryl or polymeric derivatives which have base attachment capacity.

Agents suitable for use in these methods preferably contain 20 to 40 bases and are designed to be complementary to a region of the gene involved in transcription (triple helix - see Lee et al., Nucl. Acids Res. 6:3073 (1979); Cooney et al., Science 241:456 (1988); and Dervan et al., Science 251:1360 (1991)) or to the mRNA itself (antisense - Okano, J. Neurochem. 56:560 (1991); Oligodeoxynucleotides as Antisense Inhibitors of Gene Expression, CRC Press, Boca Raton, FL (1988)). Triple helix-formation optimally results in a shut-off of RNA transcription from DNA, while antisense RNA hybridization blocks translation of an mRNA molecule into polypeptide. Both techniques have been demonstrated to be effective in model systems. Information contained in the sequences of the present invention is necessary for the design of an antisense or triple helix oligonucleotide and other DNA binding agents.

Agents which bind to a protein encoded by one of the ORFs of the present invention can be used as a diagnostic agent. Agents which bind to a protein encoded by one of the ORFs of the present invention can be formulated using known techniques to generate a pharmaceutical composition.

4.19 USE OF NUCLEIC ACIDS AS PROBES

Another aspect of the subject invention is to provide for polypeptide-specific nucleic acid hybridization probes capable of hybridizing with naturally occurring nucleotide sequences. The hybridization probes of the subject invention may be derived from any of the nucleotide sequences SEQ ID NO: 1-444. Because the corresponding gene is only expressed in a limited number of tissues, a hybridization probe derived from any of the nucleotide sequences SEQ ID NO: 1-444 can be used as an indicator of the presence of RNA of cell type of such a tissue in a sample.

Any suitable hybridization technique can be employed, such as, for example, in situ hybridization. PCR as described in US Patents Nos. 4.683.195 and 4.965.188 provides

additional uses for oligonucleotides based upon the nucleotide sequences. Such probes used in PCR may be of recombinant origin, may be chemically synthesized, or a mixture of both. The probe will comprise a discrete nucleotide sequence for the detection of identical sequences or a degenerate pool of possible sequences for identification of closely related genomic sequences.

Other means for producing specific hybridization probes for nucleic acids include the cloning of nucleic acid sequences into vectors for the production of mRNA probes. Such vectors are known in the art and are commercially available and may be used to synthesize RNA probes in vitro by means of the addition of the appropriate RNA polymerase as T7 or SP6 RNA polymerase and the appropriate radioactively labeled nucleotides. The nucleotide sequences may be used to construct hybridization probes for mapping their respective genomic sequences. The nucleotide sequence provided herein may be mapped to a chromosome or specific regions of a chromosome using well known genetic and/or chromosomal mapping techniques. These techniques include in situ hybridization, linkage analysis against known chromosomal markers, hybridization screening with libraries or flow-sorted chromosomal preparations specific to known chromosomes, and the like. The technique of fluorescent in situ hybridization of chromosome spreads has been described, among other places, in Verma et al (1988) Human Chromosomes: A Manual of Basic Techniques, Pergamon Press, New York NY.

Fluorescent in situ hybridization of chromosomal preparations and other physical chromosome mapping techniques may be correlated with additional genetic map data. Examples of genetic map data can be found in the 1994 Genome Issue of Science (265:1981f). Correlation between the location of a nucleic acid on a physical chromosomal map and a specific disease (or predisposition to a specific disease) may help delimit the region of DNA associated with that genetic disease. The nucleotide sequences of the subject invention may be used to detect differences in gene sequences between normal, carrier or affected individuals.

4.20 PREPARATION OF SUPPORT BOUND OLIGONUCLEOTIDES

Oligonucleotides, i.e., small nucleic acid segments, may be readily prepared by, for example, directly synthesizing the oligonucleotide by chemical means, as is commonly practiced using an automated oligonucleotide synthesizer.

Support bound oligonucleotides may be prepared by any of the methods known to those of skill in the art using any suitable support such as glass, polystyrene or Teflon. One strategy is to precisely spot oligonucleotides synthesized by standard synthesizers. Immobilization can be achieved using passive adsorption (Inouye & Hondo, (1990) J. Clin. Microbiol. 28(6) 1469-72); using UV light (Nagata et al., 1985; Dahlen et al., 1987; Morrissey & Collins, (1989) Mol. Cell

Probes 3(2) 189-207) or by covalent binding of base modified DNA (Keller *et al.*, 1988; 1989); all references being specifically incorporated herein.

Another strategy that may be employed is the use of the strong biotin-streptavidin interaction as a linker. For example, Broude et al. (1994) Proc. Natl. Acad. Sci. USA 91(8) 3072-6, describe the use of biotinylated probes, although these are duplex probes, that are immobilized on streptavidin-coated magnetic beads. Streptavidin-coated beads may be purchased from Dynal, Oslo. Of course, this same linking chemistry is applicable to coating any surface with streptavidin. Biotinylated probes may be purchased from various sources, such as, e.g., Operon Technologies (Alameda, CA).

Nunc Laboratories (Naperville, IL) is also selling suitable material that could be used. Nunc Laboratories have developed a method by which DNA can be covalently bound to the microwell surface termed Covalink NH. CovaLink NH is a polystyrene surface grafted with secondary amino groups (>NH) that serve as bridge-heads for further covalent coupling. CovaLink Modules may be purchased from Nunc Laboratories. DNA molecules may be bound to CovaLink exclusively at the 5'-end by a phosphoramidate bond, allowing immobilization of more than 1 pmol of DNA (Rasmussen et al., (1991) Anal, Biochem. 198(1) 138-42).

The use of CovaLink NH strips for covalent binding of DNA molecules at the 5'-end has been described (Rasmussen et al., (1991). In this technology, a phosphoramidate bond is employed (Chu et al., (1983) Nucleic Acids Res. 11(8) 6513-29). This is beneficial as immobilization using only a single covalent bond is preferred. The phosphoramidate bond joins the DNA to the CovaLink NH secondary amino groups that are positioned at the end of spacer arms covalently grafted onto the polystyrene surface through a 2 nm long spacer arm. To link an oligonucleotide to CovaLink NH via an phosphoramidate bond, the oligonucleotide terminus must have a 5'-end phosphate group. It is, perhaps, even possible for biotin to be covalently bound to CovaLink and then streptavidin used to bind the probes.

More specifically, the linkage method includes dissolving DNA in water (7.5 ng/µl) and denaturing for 10 min. at 95°C and cooling on ice for 10 min. Ice-cold 0.1 M 1-methylimidazole, pH 7.0 (1-MeIm₇), is then added to a final concentration of 10 mM 1-MeIm₇. The single-stranded DNA solution is then dispensed into CovaLink NH strips (75 µl/well) standing on ice.

Carbodiimide 0.2 M 1-ethyl-3-(3-dimethylaminopropyl)-carbodiimide (EDC), dissolved in 10 mM 1-MeIm₇, is made fresh and 25 µl added per well. The strips are incubated for 5 hours at 50°C. After incubation the strips are washed using, e.g., Nunc-Immuno Wash; first the wells are washed 3 times, then they are soaked with washing solution for 5 min., and finally they are washed 3 times (where in the washing solution is 0.4 N NaOH. 0.25% SDS heated to 50°C).

It is contemplated that a further suitable method for use with the present invention is that described in PCT Patent Application WO 90/03382 (Southern & Maskos), incorporated herein by reference. This method of preparing an oligonucleotide bound to a support involves attaching a nucleoside 3'-reagent through the phosphate group by a covalent phosphodiester link to aliphatic hydroxyl groups carried by the support. The oligonucleotide is then synthesized on the supported nucleoside and protecting groups removed from the synthetic oligonucleotide chain under standard conditions that do not cleave the oligonucleotide from the support. Suitable reagents include nucleoside phosphoramidite and nucleoside hydrogen phosphorate.

An on-chip strategy for the preparation of DNA probe for the preparation of DNA probe arrays may be employed. For example, addressable laser-activated photodeprotection may be employed in the chemical synthesis of oligonucleotides directly on a glass surface, as described by Fodor et al. (1991) Science 251(4995) 767-73, incorporated herein by reference. Probes may also be immobilized on nylon supports as described by Van Ness et al. (1991) Nucleic Acids Res. 19(12) 3345-50; or linked to Teflon using the method of Duncan & Cavalier (1988) Anal. Biochem. 169(1) 104-8; all references being specifically incorporated herein.

To link an oligonucleotide to a nylon support, as described by Van Ness et al. (1991), requires activation of the nylon surface via alkylation and selective activation of the 5'-amine of oligonucleotides with evanuric chloride.

One particular way to prepare support bound oligonucleotides is to utilize the light-generated synthesis described by Pease et al., (1994) PNAS USA 91(11) 5022-6, incorporated herein by reference). These authors used current photolithographic techniques to generate arrays of immobilized oligonucleotide probes (DNA chips). These methods, in which light is used to direct the synthesis of oligonucleotide probes in high-density, miniaturized arrays, utilize photolabile 5'-protected N-acyl-deoxynucleoside phosphoramidites, surface linker chemistry and versatile combinatorial synthesis strategies. A matrix of 256 spatially defined oligonucleotide probes may be generated in this manner.

4.21 PREPARATION OF NUCLEIC ACID FRAGMENTS

The nucleic acids may be obtained from any appropriate source, such as cDNAs, genomic DNA, chromosomal DNA, microdissected chromosome bands, cosmid or YAC inserts, and RNA, including mRNA without any amplification steps. For example, Sambrook et al. (1989) describes three protocols for the isolation of high molecular weight DNA from mammalian cells (p. 9.14-9.23).

DNA fragments may be prepared as clones in M13, plasmid or lambda vectors and/or prepared directly from genomic DNA or cDNA by PCR or other amplification methods. Samples

may be prepared or dispensed in multiwell plates. About 100-1000 ng of DNA samples may be prepared in 2-500 ml of final volume.

The nucleic acids would then be fragmented by any of the methods known to those of skill in the art including, for example, using restriction enzymes as described at 9.24-9.28 of Sambrook et al. (1989), shearing by ultrasound and NaOH treatment.

Low pressure shearing is also appropriate, as described by Schriefer et al. (1990) Nucleic Acids Res. 18(24) 7455-6, incorporated herein by reference). In this method, DNA samples are passed through a small French pressure cell at a variety of low to intermediate pressures. A lever device allows controlled application of low to intermediate pressures to the cell. The results of these studies indicate that low-pressure shearing is a useful alternative to sonic and enzymatic DNA fragmentation methods.

One particularly suitable way for fragmenting DNA is contemplated to be that using the two base recognition endonuclease, CviII, described by Fitzgerald et al. (1992) Nucleic Acids Res. 20(14) 3753-62. These authors described an approach for the rapid fragmentation and fractionation of DNA into particular sizes that they contemplated to be suitable for shotgun cloning and sequencing.

The restriction endonuclease CviJI normally cleaves the recognition sequence PuGCPy between the G and C to leave blunt ends. Atypical reaction conditions, which alter the specificity of this enzyme (CviJI**), yield a quasi-random distribution of DNA fragments form the small molecule pUC19 (2688 base pairs). Fitzgerald et al. (1992) quantitatively evaluated the randomness of this fragmentation strategy, using a CviJI** digest of pUC19 that was size fractionated by a rapid gel filtration method and directly ligated, without end repair, to a lac Z minus M13 cloning vector. Sequence analysis of 76 clones showed that CviJI** restricts pyGCPy and PuGCPu, in addition to PuGCPy sites, and that new sequence data is accumulated at a rate consistent with random fragmentation.

As reported in the literature, advantages of this approach compared to sonication and agarose gel fractionation include: smaller amounts of DNA are required (0.2-0.5 µg instead of 2-5 µg); and fewer steps are involved (no preligation, end repair, chemical extraction, or agarose gel electrophoresis and elution are needed

Irrespective of the manner in which the nucleic acid fragments are obtained or prepared, it is important to denature the DNA to give single stranded pieces available for hybridization. This is achieved by incubating the DNA solution for 2-5 minutes at 80-90°C. The solution is then cooled quickly to 2°C to prevent renaturation of the DNA fragments before they are contacted with the chip. Phosphate groups must also be removed from genomic DNA by methods known in the art.

4.22 PREPARATION OF DNA ARRAYS

Arrays may be prepared by spotting DNA samples on a support such as a nylon membrane. Spotting may be performed by using arrays of metal pins (the positions of which correspond to an array of wells in a microtiter plate) to repeated by transfer of about 20 nl of a DNA solution to a nylon membrane. By offset printing, a density of dots higher than the density of the wells is achieved. One to 25 dots may be accommodated in 1 mm², depending on the type of label used. By avoiding spotting in some preselected number of rows and columns, separate subsets (subarrays) may be formed. Samples in one subarray may be the same genomic segment of DNA (or the same gene) from different individuals, or may be different, overlapped genomic clones. Each of the subarrays may represent replica spotting of the same samples. In one example, a selected gene segment may be amplified from 64 patients. For each patient, the amplified gene segment may be in one 96-well plate (all 96 wells containing the same sample). A plate for each of the 64 patients is prepared. By using a 96-pin device, all samples may be spotted on one 8 x 12 cm membrane. Subarrays may contain 64 samples, one from each patient. Where the 96 subarrays are identical, the dot span may be 1 mm² and there may be a 1 mm space between subarrays.

Another approach is to use membranes or plates (available from NUNC, Naperville, Illinois) which may be partitioned by physical spacers e.g. a plastic grid molded over the membrane, the grid being similar to the sort of membrane applied to the bottom of multiwell plates, or hydrophobic strips. A fixed physical spacer is not preferred for imaging by exposure to flat phosphor-storage screens or x-ray films.

The present invention is illustrated in the following examples. Upon consideration of the present disclosure, one of skill in the art will appreciate that many other embodiments and variations may be made in the scope of the present invention. Accordingly, it is intended that the broader aspects of the present invention not be limited to the disclosure of the following examples. The present invention is not to be limited in scope by the exemplified embodiments which are intended as illustrations of single aspects of the invention, and compositions and methods which are functionally equivalent are within the scope of the invention. Indeed, numerous modifications and variations in the practice of the invention are expected to occur to those skilled in the art upon consideration of the present preferred embodiments. Consequently, the only limitations which should be placed upon the scope of the invention are those which appear in the appended claims.

All references cited within the body of the instant specification are hereby incorporated by reference in their entirety.

5. EXAMPLES

51 EXAMPLE 1

Novel Nucleic Acid Sequences Obtained From Various Libraries

A plurality of novel nucleic acids were obtained from cDNA libraries prepared from various human tissues and in some cases isolated from a genomic library derived from human chromosome using standard PCR, SBH sequence signature analysis and Sanger sequencing techniques. The inserts of the library were amplified with PCR using primers specific for the vector sequences which flank the inserts. Clones from cDNA libraries were spotted on nylon membrane filters and screened with oligonucleotide probes (e.g., 7-mers) to obtain signature sequences. The clones were clustered into groups of similar or identical sequences. Representative clones were selected for sequencing.

In some cases, the 5' sequence of the amplified inserts was then deduced using a typical Sanger sequencing protocol. PCR products were purified and subjected to fluorescent dye terminator cycle sequencing. Single pass gel sequencing was done using a 377 Applied Biosystems (ABI) sequencer to obtain the novel nucleic acid sequences

5.2 EXAMPLE 2

Assemblage of Novel Nucleic Acids

The nucleic acids of the present invention, designated as SEQ ID NO: 1-444 were assembled using an EST sequence as a seed. Then a recursive algorithm was used to extend the seed EST into an extended assemblage, by pulling additional sequences from different databases (i.e., Hyseq's database containing EST sequences, dbEST, gb pri, and UniGene, and exons from public domain genomic sequences predicated by GenScan) that belong to this assemblage. The algorithm terminated when there was no additional sequences from the above databases that would extend the assemblage. Further, inclusion of component sequences into the assemblage was based on a BLASTN hit to the extending assemblage with BLAST score greater than 300 and percent identity greater than 95%.

Using PHRAP (Univ. of Washington) or CAP4 (Paracel), full-length gene sequences and their corresponding protein sequences were generated from the assemblage. Any frame shifts and incorrect stop codons were corrected by hand editing. During editing, the sequence was checked using FASTXY algorithm against Genbank (i.e., dbEST, gb pri, UniGene, and Genpept). Other computer programs which may have been used in the editing process were phredPhrap and Consed (University of Washington) and ed-ready, ed-ext and gc-zip-2 (Hyseq, Inc.). The full-length nucleotide sequences are shown in the Sequence Listing as SEQ ID NO: 1-444. The corresponding polypeptide sequences are SEQ ID NO: 445-888.

Table 1 shows the various tissue sources of SEQ ID NO: 1-444.

The nearest neighbor results for polypeptides encoded by SEQ ID NO: 1-444 (i.e. SEQ ID NO: 445-888) were obtained by a BLASTP (version 2.0al 19MP-WashU) search against Genpept release 124 using BLAST algorithm. The nearest neighbor result showed the closest homologue with functional annotation for SEQ ID NO: 1-444 from Genpept. The translated amino acid sequences for which the nucleic acid sequence encodes are shown in the Sequence Listing. The homologues with identifiable functions for SEQ ID NO: 1-444 are shown in Table 2 below.

Using eMatrix software package (Stanford University, Stanford, CA) (Wu et al., J. Comp. Biol., Vol. 6 pp. 219-235 (1999) herein incorporated by reference), polypeptides encoded by SEQ ID NO: 1-444 (i.e. SEQ ID NO: 445-888) were examined to determine whether they had identifiable signature regions. Table 3 shows the signature region found in the indicated polypeptide sequences, the description of the signature, the eMatrix p-value(s) and the position(s) of the signature within the polypeptide sequence.

Using the pFam software program (Sonnhammer et al., Nucleic Acids Res., Vol. 26(1) pp. 320-322 (1998) herein incorporated by reference) polypeptides encoded by SEQ ID NO: 1-444 (i.e. SEQ ID NO: 445-888) were examined for domains with homology to certain peptide domains. Table 4 shows the name of the domain found, the description, the p-value and the pFam score for the identified domain within the sequence.

The GeneAtlas™ software package (Molecular Simulations Inc. (MSI), San Diego, CA) was used to predict the three-dimensional structure models for the polypeptides encoded by SEQ ID NO: 1-444 (i.e. SEO ID NO: 445-888). Models were generated by (1) PSI-BLAST which is a multiple alignment sequence profile-based searching developed by Altschul et al. (Nucl. Acids. Res. 25, 3389-3408 (1997)), (2) High Throughput Modeling (HTM) (Molecular Simulations Inc. (MSI) San Diego, CA.) which is an automated sequence and structure searching procedure (http://www.msi.com/), and (3) SegFold™ which is a fold recognition method described by Fischer and Eisenberg (J. Mol. Biol. 209, 779-791 (1998)). This analysis was carried out, in part, by comparing the polypeptides of the invention with the known NMR (nuclear magnetic resonance) and x-ray crystal three-dimensional structures as templates. Table 5 shows, "PDB ID", the Protein DataBase (PDB) identifier given to template structure; "Chain ID", identifier of the subcomponent of the PDB template structure; "Compound Information", information of the PDB template structure and/or its subcomponents: "PDB Function Annotation" gives function of the PDB template as annotated by the PDB files (http://www.rcsb.org/PDB/); start and end amino acid position of the protein sequence aligned; PSI-BLAST score, the verify score, the SeaFold score, and the Potential(s) of Mean Force (PMF). The verify score is produced by GeneAtlas™

software (MSI), is based on Dr. Eisenberg's Profile-3D threading program developed in Dr. David Eisenberg's laboratory (US patent no. 5,436,850 and Luthy, Bowie, and Eisenberg, Nature, 356:83-85 (1992)) and a publication by R. Sanchez and A. Sali, Proc. Natl. Acad. Sci. USA, 95:13597-12502. The verify score produced by GeneAtlas normalizes the verify score for proteins with different lengths so that a unified cutoff can be used to select good models as follows:

Verify score (normalized) = (raw score - 1/2 high score)/(1/2 high score)

The PFM score, produced by GeneAtlas™ software (MSI), is a composite scoring function that depends in part on the compactness of the model, sequence identity in the alignment used to build the model, pairwise and surface mean force potentials (MFP). As given in table 8, a verify score between 0 to 1.0, with 1 being the best, represents a good model. Similarly, a PMF score between 0 to 1.0, with 1 being the best, represents a good model. A SeqFold™ score of more than 50 is considered significant. A good model may also be determined by one of skill in the art based all the information in Table 5 taken in totality.

The nucleotide sequence within the sequences that codes for signal peptide sequences and their cleavage sites can be determined from using Neural Network SignalP V1.1 program (from Center for Biological Sequence Analysis, The Technical University of Denmark). The process for identifying prokaryotic and eukaryotic signal peptides and their cleavage sites are also disclosed by Henrik Nielson, Jacob Engelbrecht, Soren Brunak, and Gunnar von Heijne in the publication "Identification of prokaryotic and eukaryotic signal peptides and prediction of their cleavage sites" Protein Engineering, Vol. 10, no. 1, pp. 1-6 (1997), incorporated herein by reference. A maximum S score and a mean S score, as described in the Nielson et al, as reference, were obtained for the polypeptide sequences. Table 6 shows the position of the last amino acid of the signal peptide in each of the polypeptides and the maximum score and mean score associated with that signal peptide.

Table 7 correlates each of SEQ ID NO: 1-444 to a specific chromosomal location.

Table 8 is a correlation table of the novel polynucleotide sequences SEQ ID NO: 1-444, and their corresponding priority nucleotide sequences in the priority application USSN 09/659,671, herein incorporated by reference in its entirety.

TABLE 1

| Tissue Origin | RNA Source | Library | SEO ID NO: |
|-----------------|--------------|---------|---|
| rissuc Origin | IC TA Source | Name | SEQ ID NO. |
| adult brain | GIBCO | AB3001 | 4 6-8 12 23 33-34 47 50 55 57-60 62 89 102 |
| | | | 104-106 123 144 162 176-177 179 187 194 |
| | | | 248 260 270 279 292 294 297-298 307 322- |
| | | | 323 326 333 336 341 351 450 |
| adult brain | GIBCO | ABD003 | 6 10 12-15 17-18 26 31 34-35 38-40 42-44 |
| | | | 46 48-50 53 56 59-60 64 66 70-72 80-81 |
| | | | 85-86 98 101 107 116-117 125 130 138-139 |
| | | | 142 144 147 151 160-161 164 173 175-177 |
| ľ | | 1 | 179 184-185 187-188 194-195 198 201 215 |
| | | | 217-218 222 226 228 232 239-240 243-244 |
|) | ļ. | } | 247 252 256 258 260 264-265 267 274-275 |
| | | | 284 288 290 293 298 306-308 314-315 318- |
| | | | 320 325-326 333-334 337 341 343 345-346 |
| | | | 351-354 364-365 371 390-391 424-425 429 |
| adult brain | Clontech | ABR001 | 5 36 43 76 108 128 182-183 212 239 242 |
| | Clontech | 1 DDOOC | 260 263 269 296 325 351 364 371-372 423 2 9 11 13 18 23 35 38 42 46 50-51 53-54 60 |
| adult brain | Ciontecn | ABR006 | 63 66 85 91 107-108 116-117 120 122 128 |
| | | | 170 178 180 184 187-188 193-194 198 202 |
| | | - | 215 232 243 245 257-258 260 266-267 271 |
| | ľ | ļ | 285 294 301 333-334 337 370 389 394-396 |
| | | i | 400 405 412 423 428 434 436 453 458 |
| adult brain | Clontech | ABR008 | 1 3 7 10-14 16-17 19-23 26-28 34-35 38-39 |
| | | | 41 43 46-48 51-54 56 60 62 64 66-68 75 82 |
| ! | | | 86-87 91 96-98 102 104-106 108 110-111 |
| | | | 114 116-118 122 125 127-130 134 138-139 |
| 1 | | | 141-143 145-146 150-151 153 156 158 160 |
| 1 | 1 | Į. | 162 167-170 173-175 177-180 182 185-186 |
| | | | 191-194 196-197 200-201 205-206 208-209 |
| 1 | | ŀ | 211 213-215 219-220 226-227 231 238 241 |
| - | ì | | 244 246-248 252 256 260 262-265 269 271 |
| | | | 273 278-280 282 284 290 292 296 298 301- |
| i | 1 | ł | 302 306 309 311 315-317 322-323 325-327 |
| | | ł | 329-331 335-337 339 342-343 345-346 |
| | | l . | 350-355 359-360 362 364 368 370 372 374 376 381 383 385 387 390-395 400-401 405 |
| | | | 410 412 414 417 420-421 423-425 432 440 |
| 1 | 1 | ļ | 447 450-452 459 472-473 |
| adult brain | Clontech | ABR011 | 174 177 360 |
| adult brain | BioChain | ABR012 | 334 341 |
| adult brain | BioChain | ABR013 | 41-42 60 101 163 355 |
| adult brain | Invitrogen | ABR014 | 53 95 104-106 143 149 177 180 258 |
| adult brain | Invitrogen | ABR015 | 42 70-72 79 95 112 138-140 163 195 275 |
| . addit orani | mvinogon | ADIOUS | 288 322-323 341 343 458 |
| adult brain | Invitrogen | ABR016 | 13 31 60 79 124 136 154 163 333 341 343 |
| door oran | III TI GOOD | 7124010 | 364 370 |
| adult brain | Invitrogen | ABT004 | 1 11-13 15 18 24-26 34 50 56 68 87 98 104- |
| Lucia orani | | 1.2.00 | 106 111 123-124 131-133 137 144 146 173 |
| | | l . | 189 194 206 224 247-248 260 262 264 269 |
| | 1 | 1 | 272 274 282 298 318 327 335 346 351 356- |
| | | - | 357 372 375 381 392 409-410 421 |
| cultured | Stratagene | ADP001 | 2 11-14 24-25 40 42 47 50 52 57-58 69 76 |
| preadipocytes . |] | | 107 120 144 151 156 163 168 171 194 197 |
| 1 | | | 199 203-204 215 229 250-251 262 294 333 |
| | | | 338 341 415 450 469-473 |
| adrenal gland | Clontech | ADR002 | 10-11 16 18 22-23 27-28 33-35 40 43-45 49 |
| 1 | | | |
| | | | 61 66 85 98 107-108 111 116-117 124 136 143 145 160 167 173 175 184 187 201 217- |

| | | 10. | |
|----------------------------|------------------------|------------------|---|
| | | | 218 229 249-251 258 262 269 271 273 277 280 287 289 298 301 308 322-323 337 352 354 360 414 425 445-446 463 |
| adult heart | GIBCO | AHR001 | 11-13 15 20-23 26-27 30 33-34 37-40 49 53 36-58 62-65 67-68 76-77 86 86 89 53-94 101 104-108 112 114 116-117 119 121-125 128-130 142 144-145 148 150 154-156 164-165 167 174-176 178-179 182 184 186-187 189 195 198 200 202 210 213-219 |
| | 3 | | 221 228-229 235 238 240 242-243 246-247 252-253 260 262 264 266-267 269 275 278 280-281 283 286-289 293-294 297 302-304 308 311 313 315-316 318-320 322-324 328-331 333 336 340-341 343 347 355-356 359 380-382 386-388 413-414 436 |
| adult kidney | GIBCO | AKD001 | 4-5 8-13 15-18 20-27 33-35 37 39 42 45-48 49 52-54 56-59 62 65-67 73 75 77 80-18 83 85-86 88 91 97-98 100-108 112 117 119 122 124-125 127-129 134 138-412 145-146 151 153 155 158 160 162 164-165 168 170 174-176 178-181 186-189 190-199 202 209 211-121 215-216 222 232 255 237-240 244 246-248 250-252 257-258 260 262 264 269-271 275 280 282-284 287-289 291-294 297 303-312 314-317 322-323 325 327-329 333 336-337 341 357 359 375 403 407-408 413 428 436 469-471 |
| adult kidney | Invitrogen | AKT002 | 1 10-11 13 17-18 26-27 35 42 54 64 66 73 77 82 87 91 94 96-97 113-114 118 135 146 148 160 173-174 182 187 196 198 200 218- 219 221 239 243-244 249-251 257-258 260 264 269-270 274-272 584-285 287-288 260 302-303 308-309 312 322-324 330 332-333 335-337 344 346 369 402 404 417 425 428 447 462 |
| adult lung | GIBCO | ALG001 | 4 6 17-18 24-26 39 43-44 46 49 51 53 55 57-58 76 84 90 95 98 107 111 126 150 155 157 164 173 176 184 187 195 210 248-249 252-253 261 264 275 278 281 287 306 309 312 314 322-323 333 338 340-341 352 358 365 372 403 450 |
| lymph node | Clontech | ALN001 | 17 19 26 81 85 149 166 218 228 260 264 275-276 282 321 333 341 395-396 436 |
| young liver | GIBCO | ALV001 | 10 12 14 16-18 20 22 33 40 46 48 56 73 82 85 88 100 102 117 126 134 142-143 173 175 182 197 209 220 237-239 243 246-247 279 290 294 302 306 309 319-320 327 334 359 |
| adult liver | Invitrogen | ALV002 | 10 15 22 24-25 33 49 66 75 86 95 109 111 130 138-139 148 151 156 187 189 222 237- 238 246 249 274 282 286 290 298 301 333 371 377 387 395 424-425 430 |
| adult liver adult ovary | Clontech Invitrogen | ALV003 AOV001 | 73 92 294 341 14 6-18 23 27-28 30-34 39 42-47 49-50 52-59 61-62 64-68 75-77 79 81-82 85-88 90 93-96 98 100-107 109-111 13-115 117 12 123 125-129 134-136 140 142-145 148 15 1 54 156 158 160-146 169-171 175-176 176-179 181-184 187-188 194-196 200 202-304 206 209-210 12 1214-215 217-220 202-242 27 229 233 235 238-240 242-244 |

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| | | | 275 277-281 283-284 287-294 296-298 |
| | | Į | 301-304 306-308 310-311 313-316 318-326 |
| | | | 328-330 333-342 344 346 349 352-353 |
| | | | 356-358 360-361 363 369 372 375 382-383 |
| | | | 395-396 402-403 405-407 409 415 417-419 |
| | L | | 421 425-427 435-436 450 456 467 469-473 |
| adult placenta | Invitrogen | APL001 | 17 33 157 228 232 264 |
| placenta | Invitrogen | APL002 | 11-12 23 31 35 51 53 88 104-106 138-139 |
| | | | 151 260 279 296 307 327 334 337 |
| adult spleen | GIBCO | ASP001 . | 1 5 11 14 18-20 22-23 33-34 39-40 48-49 |
| | 1 | | 56-59 62 65 87 91 95 98 104-106 108-109 113-115 124 128 142 145 149-150 158 162- |
| | | | 163 173 195 198 202 210 224 227 232 250- |
| | | | 251 253 264 275 277 281 285-286 299 321 |
| | | | 333 399 |
| - d. It to - d'- | GIBCO | ATS001 | 8 10-11 13 17 28 43-44 49 54 57-59 62 77 |
| adult testis | GIBCO | A15001 | 109 134 138-139 143-144 148 156 163-164 |
| | | | 174 178 182 187-188 200 202 206 216 221 |
| | | 1 | 232 243 258 290 292 294 297-298 304 308- |
| | | ĺ | 309 324 333 336-337 339-341 346 425 472- |
| | 1 | ļ | 473 |
| adult bladder | Invitrogen | BLD001 | 11 24-25 44 57-58 65 141 150-151 163 187 |
| adult bladder | Invitrogen | BLDOOL | 195 222 224 244-245 247 260 263 277 282 |
| | | ì | 334 356 369 375 390-391 416 425 472-473 |
| bone marrow | Clontech | BMD001 | 9 11 13-14 17 19 22-23 27-28 30 32-35 38 |
| oone marrow | Cioniccii | DIVIDUOI | 42 46 48-49 51 56-58 62-63 68 74-76 78 80 |
| | | | 84-85 87 89 91 93 95 97-98 102 104-106 |
| | 1 | | 108 111-112 114-115 117 121-122 125 |
| | 1 | | 138-140 143 146 149 151 154-155 157-171 |
| | 1 | | 174 176 179 184 187 190 195 200 202 205- |
| | | 1 | 206 210 215 218-222 224-236 239 249 258 |
| | 1 | ł | 262 264 269 285 294 297 304 310 319-321 |
| | | | 324-325 331 333 341-342 363 420 450 |
| bone marrow | Clontech | BMD002 | 1 5 7 10-11 14 16 19-20 23-25 28 30-31 35 |
| | | | 40 42-43 46 48-49 51 54 56 62 64 68 74 77 |
| | | | 87 89 91 93-96 98-99 104-106 108 110 |
| | | į. | 114-115 117 121-122 128 138-139 141 143 |
| | | | 145-146 149-151 156-158 163 165 169-171 |
| | | 1 | 174 178-179 181 195 199 203-206 210 212 |
| | | | 216 218 220-221 224 234-235 240 245 248- |
| | 1 | | 252 254-255 258-260 262 264 269 276-278 |
| | | | 285 292 302-303 308-309 312 322-324 326 |
| | | | 333 341 343 346 350 352 355 362 379 384- |
| | | | 386 394 410 418 420 425 440-441 449-451 |
| -, | | | 469-474 |
| bone marrow | Clontech | BMD004 | 97 149 |
| bone marrow | Clontech | BMD007 | 53 143 149 221 |
| colon | Invitrogen | CLN001 | 10 34 49 52-53 57-59 145 163 175 197 238 |
| | <u> </u> | COTT O.L.C | 246-247 315-316 346 364 442 |
| mixture of 16 | various vendors | CTL016 | 10 56 |
| tissues/mRNAs | | COTT DO 1 | 140 |
| mixture of 16 | various vendors | CTL021 | 149 |
| tissues/mRNAs | | CTL028 | 145 358 |
| mixture of 16 | various vendors | C1L028 | 143 330 |
| tissues/mRNAs | DisChain | CVX001 | 1 4 6 11 23-25 27 30 34-35 39-40 46 50 59 |
| adult cervix | BioChain | CAYOU | 62-64 76-77 80-81 88 93 100 107 111-112 |
| | 1 . | | 116 118-119 122-123 125 136 138-139 143 |
| | | 1 | 146 151 155 160 163 176 178-182 184 188 |
| | | | 195 209 215 218 221 228 232-233 235 239- |
| | | | 240 250-251 261-262 264 266 278 283 287- |
| | | | 288 300 306-308 311 319-320 322-323 325 |
| | | | 1 200 500 500 500 511 517 520 522 525 520 |

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|--------------------|------------|--------|---|
| | | 1 | 329 333 337 341 349 361 369 388 397 403 |
| | | | 407 422 425 429-430 435-436 453 469-471 |
| endothelial cells | Stratagene | EDT001 | 1 4 6-8 10-14 16-28 31 34-35 37 39 42-44 46 49 51 53-54 56-59 62-63 66 70-72 76-78 |
| | i | | 80-81 83-84 88 96 101 104-107 110 114 |
| | i | | 116 118-119 122-124 130 134 136 138-140 |
| | | l | 143-146 153-155 158 160 162-163 170 |
| | ł | l | 174-175 184 186-187 189 194-195 197 200 |
| | | 1 | 203-204 209-210 212 214-217 219 222-223 |
| | | 1 | 229 232-233 235-238 240 242 244 246-248 |
| | l * | | 250-251 253 256 258 260-262 264 267 269- |
| | | | 270 272 276-277 279-282 284-285 288-292 |
| | l . | | 294 302-304 308 312 317 319-320 324-325 |
| · ' | 1 | | 329 333-334 336-337 339 341 361 375 378 |
| | | | 384-385 397 404 411 415-416 450 469-473 |
| fetal brain | Clontech | FBR001 | 46 104-106 175 193 258 341 |
| fetal brain | Clontech | FBR004 | 193-194 226-227 229 260 264 334 |
| fetal brain | Clontech | FBR006 | 2-3 9-12 14 16-17 19-20 23 27-28 39 43 52- |
| | i | | 53 59 66-67 76 86 91-92 94-95 97-98 101- |
| | | | 102 104-108 110-111 116-117 125 127-130 |
| | | | 134 138-139 142-143 145-148 150-151 167 |
| | | | 170 174-175 178-179 185 187 194 198 200- |
| | | | 201 212 215 226-228 231 241 245 261 264 |
| i | | l | 269 276-277 279 281-282 284 290 292 300 |
| | | | 302 309 325 327 331 333-334 336-337 345 |
| | | | 350-353 357 362 371 376 382-383 388-389 |
| | | | 392 395-396 399 401 414 420 427 432 453 |
| | <u> </u> | | 456 458 472-473 |
| fetal brain | Clontech | FBRS03 | 199 291 402 |
| fetal brain | Invitrogen | FBT002 | 12 15 19-20 23 30-31 47 53 59 76 86 94 99 |
| | l . | 1 | 104-107 128 131-133 136 144 148 150 163 |
| | | | 168 173 175 185 201 220 233 244 250-251 254-255 262 273 282 307 309 315-316 322- |
| | | | 323 327 334-335 337 341 351 364 375 392 |
| | | 1 | 409-412 421 423 469-473 |
| fetal heart | Invitrogen | FHR001 | 34 43 81 87 129 134 138-139 145 200 288- |
| tetai neart | Hivitrogen | FIROUI | 289 304 315-316 392 |
| fetal kidney | Clontech | FKD001 | 6 8 10 17 50 54 77 86 92 112 114 179 217 |
| Iciai kidiley | Cioniccii | 110001 | 223 241 269 301 319-320 322-323 333 340- |
| | ł | | 341 397-398 |
| fetal kidney | Clontech | FKD002 | 141 264 309 341 432 |
| fetal kidney | Invitrogen | FKD007 | 107 123 |
| fetal lung | Clontech | FLG001 | 16 33 92 100 149 257 337 340 396 |
| fetal lung | Invitrogen | FLG003 | 8 13 15 32 39 48 51 56 91-93 130-133 146 |
| | | 1 | 148 197-198 222 244 257 262 280 286 294 |
| | | | 302 315-316 327 337 352 364 392 396 440 |
| fetal lung | Clontech | FLG004 | 122 209 |
| fetal liver-spleen | Columbia | FLS001 | 1-13 15-46 48-51 53 55 57-59 61-95 97-119 |
| • | University | | 121-136 138-139 141 143 146-155 158 160 |
| | | | 162-165 167 169-171 178 184 186-187 189 |
| | | | 195 209 211-212 214 219-221 223 227-229 |
| | | ł | 234-252 254-265 267-269 272-280 283 288 |
| | 1 | 1 | 290-291 295-299 302 304 307 312-317 |
| 1 | 1 | 1 | 322-323 333 341 343-344 352-353 361 |
| | | | 365-367 371 390-391 402 418 441 444 466 |
| | | | 469-473 |
| fetal liver-spleen | Columbia | FLS002 | 1-3 5 11-13 15-18 20-22 24-25 27 29-31 |
| | University | 1 | 33-34 36-40 43-44 46 49 51 53-54 56-59 61 |
| i | | 1 | 63-65 67-68 73 75 77 80-81 84-86 88-90 |
| | | 1 | 92-95 97-98 100 103 107-109 111 114 119 121-122 124 126-127 129-134 138-139 |
| | | 1 | 141-146 149 151-153 157-160 162 164-165 |
| L | L | L | 141-140 149 131-133 137-100 102 104-103 |

| fetal muscle | Invitrogen | FMS001 | 11-12 44 76 110-111 145 148-149 178 187 226 258 260 262 264-265 290 341-342 400- |
|----------------------------|------------|------------------|---|
| | 1 | | 401 404 456 |
| fetal muscle | Invitrogen | FMS002 | .8 11 23 46 52 61 102 111 120 130 134 148 |
| | | Į. | 150 170 226 233 292 318 334 355 365 386 414 418 475 |
| fetal skin | Invitrogen | FSK001 | 5-6 8 10 12 23 26-29 32-33 40 42 48-50 53 |
| | | | 55-56 59 64 67 69-72 76 83 88 98-99 102 |
| | | i | 143 148 160 163 167 174-175 195 209-210 |
| | l | | 220-221 223-224 227 237-238 240 244-247 |
| | | | 254-255 257-258 262-263 269 277 280-282 288 290-291 294-295 298-299 307 309 |
| | | \· | 322-323 327 330 333 336-337 340-341 346 |
| | | Ì | 361 364 375 387 404 408 428 432 434-435 443 448-449 452 454 |
| fetal skin | Invitrogen | FSK002 | 9 14 22 34-35 39-40 56 73 104-106 109 |
| | 1227110 | | 142-143 150 160 211 220-221 235 240 249 |
| fetal spleen | BioChain | FSP001 | 259 270 302 330 431 448 450 460 276 |
| umbilical cord | BioChain | FUC001 | 4-6 8 11 13 16 18 21-25 27 32 35 37 39-40 |
| | -100111111 | | 42 45 54 61 63 65-66 68 82 88 92-94 97 |
| | 1 | | 100-101 103-106 123 128-129 136 138-139 |
| | 1 | | 195 218 220 224 232-233 237 240-241 244 |
| | 1 | l | 247 249 262 267 277 280 284 288 291 294 |
| | | | 297-299 306 314 325 329 333-335 339 341 |
| | | - | 345 350 352 362 365 369-370 390-391 396- 397 416 472-473 |
| fetal brain | GIBCO | HFB001 | 3-4 6 11 13-14 18-20 22-23 26-27 34 37 42 |
| | | | 50 54-58 60 62-65 67 70-72 78 80-81 83-84 |
| | | | |
| | | | 87 93 98 101-107 111-112 114 116 118 123 |
| | | | 87 93 98 101-107 111-112 114 116 118 123 125 129 131-145 147 151 154 156 162-165 |
| | | | 87 93 98 101-107 111-112 114 116 118 123 |
| | | | 87 93 98 101-107 111-112 114 116 118 123 125 129 131-145 147 151 154 156 162-165 172-173 175-180 182-191 193-195 197-206 208-217 223 227 233 239-240 242-244 247 258-259 261 264 267 269 273 277 282 286 |
| | | | 87 93 98 101-107 111-112 114 116 118 123 125 129 131-145 147 151 154 156 162-165 172-173 175-180 182-191 193-195 197-206 208-217 223 227 233 239-240 242-244 247 258-259 261 264 267 269 273 277 282 286 288 290 301-302 306 310 313 325 333-334 |
| | | | 87 93 98 101-107 111-112 114 116 118 123 125 129 131-145 147 151 154 156 162-165 172-173 175-180 182-191 193-195 197-206 208-217 223 227 233 239-240 242-244 247 258-259 261 264 267 269 273 277 282 286 288 290 301-302 306 310 313 325 333-334 336-337 341 343 345 335 31 364 369-372 469- |
| macrophage | Invitrogen | HMP001 | 87 93 98 101-107 111-112 114 116 118 123 125 129 131-145 147 151 154 156 162-165 172-173 175-180 182-191 193-195 197-206 208-217 223 227 233 239-240 242-244 247 258-259 261 264 267 269 273 277 282 286 288 290 301-302 306 310 313 325 333-334 |
| macrophage infant brain | Columbia | HMP001 IB2002 | 87 93 98 101-107 111-112 114 116 118 123 125 129 131-145 147 151 154 156 162-165 172-173 175-180 182-191 193-195 197-206 208-217 223 227 233 239-240 242-244 247 258-259 261 264 267 269 273 277 282 266 288 290 301-302 306 310 313 325 333-334 343 345 351 364 369-372 469-473 49 123 144 151 275 7-8 11-13 16 20-22 24-26 34 38 44-58 60 |
| | | | 87 93 98 101-107 111-112 114 116 118 123 125 129 131-145 147 151 134 156 162-165 172-173 175-180 182-191 193-195 197-206 208-217 223 227 233 239-240 242-244 247 258-259 261 264 267 265 273 277 262 286 288 290 301-302 306 310 313 325 333-334 334 334 334 335 337 345 345 245 469-473 473 134 344 151 275 |

| | | | 175 177-178 180 182 187-188 194 196-198 200-201 206 212 15 217 219 226 232-233 239 241 247-248 255 620 623 625 626 8273 277-278 282-284 286 288-289 294 298 301-303 306-307 309 312 324 330 334-335 337-339 342-343 346-347 351 355 364 370 373-375 389-394 400 413 421 423 424 424 458 469-471 |
|--|------------------------|--------|---|
| infant brain | Columbia University | IB2003 | 4 8 11 13-14 16 23 42 46-47 50 54 56-62 65-66 76 94 98 102 119-120 135 142-143 145 150-152 158 163-164 173 175 180 226 233 244 247 260 262 267 277 302 304 309 319-320 334-337 351 364 375 383 389-392 400 423 427 454 472-473 |
| infant brain | Columbia University | IBM002 | 33 50 54 112 131-133 163 173 215 226 267 331 423 |
| infant brain | Columbia University | 1BS001 | 2 5 11 26 34 52 87 91 98 108 170 173 177 194 200-201 248 277 340 361 412 423 |
| lung, fibroblast | Stratagene | LFB001 | 13 16-17 22 26 39 46 57-58 78 83 88 93 101 116 122 131-133 160 170 178 195 198 210 214 223 262 267 276 304 319-320 322- 323 333 341 349 375 383 417 447 455 |
| lung tumor | Invitrogen | LGT002 | 10-12 15 17-18 20 23 26-28 30 32 34 37 39-40 43 49 51 56-58 62 46 68 80 85-87 91 94 98 101-102 104-106 108 111 122 124 126-129 134 136 142-144 147 156-157 168 173-176 179 184 186-187 189 195 197-198 203-204 209-210 218 220-222 226 232-233 2-339 244-246 249-251 233 257 259 259 273 277-279 282-284 287 300-301 308 310 314 319-320 327 333-335 31 346 348 352 358 362 369 371 377-379 392 394 397 406-407 410 14 241 242 244 649-471 |
| lymphocytes | ATCC | LPC001 | 7 10-11 14-15 18 20 24-25 27 33 35 43-44 49 57-58 65-67 47-58 08 89 51 03-106 108 113 116 124 130-133 145-146 151 163-164 167-171 185 200 206 215 218 226 228 223 241 244 247-248 262 267 273 275-277 284 297 321 331 345 349 352 375 400 472-473 |
| leukocyte | GIBCO . | LUC001 | 1 6-8 11 14-15 17-18 20 23-25 27-35 39 43 44 49 52-35 57-58 62-63 74 76-78 80-81 81 48-85 88 90 92-95 98 102 104-106 108 112 114 117 119 123-125 128 130-135 141 144 116 1123-125 128 130-135 141 144 116 115 133 156-158 150-164 166-168 171 174-176 178-179 18 1 83-184 187-181 187 187-200 202-204 206 209 211-216 218-219 221-232 256-228 232-235 239-240 242 244-254 247 255 258 250-256 264 256-267 270 275-277 279-280 282 284-290 292-293 297-298 300-303 63 08-81 03 12 314 317-328 330 333 335 341 346 349 400 412 427 346-347 340 464 69-473 |
| leukocyte . | Clontech | LUC003 | 17 19 27 34 42-43 46 49 90 98 104-106 108 113 122-123 128 157 206 284-285 321 333 341 362 472-473 |
| Melanoma from cell line ATCC #CRL 1424 | Clontech | MEL004 | 511 30 34 45 54-55 61-62 65-66 78 81 93 112 114 116 122 128 130 135 143 145 160 164 177 180 187 195 219 227 235 239-240 258 264-265 279-280 287 302 304 306 311 325 333 341 343 377 408 432 |
| mammary gland | Invitrogen | MMG001 | 1 5 8 10-13 15-16 18 20 24-26 30-31 34 39- |

| 40 43 45 47 49-51 53-54 57-58 62 64 66 70-72 76 80 83 87-88 95-96 99-90 101-102 104-106 108-109 112 118 124-125 127-133 136 138-139 134-2146 148 150-151 163 167 170-171 175 180 186-187 189 197 200 212 224 226-227 24 124 427-482 285-225 165 269 272 276-280 282-283 288 290 301 306-307 309 313 315-316 322-233 326-327 333-334 337 341 343-344 535 563 163 64 370 387 390-392 131 315-316 322-232 326-327 333-334 337 341 343-344 535 563 163 64 370 387 390-392 140 409 412 415 421 428 430-432 469-473 157 202 218-219 223 247 264 267 269 302 312-313 339 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 444 181 21-313 319 382 427 427 31 181 319 319 319 319 319 319 319 319 319 31 | | | | |
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| 104-106 108-109 112 118 124-125 127-133 136 138-139 142-1461 481 150-151 163 167 170-171 175 180 186-187 189 197 200 212 224 226-227 241 244 247-248 250-251 253-255 257-258 306 262-263 265 269 272 276-280 282-283 288 290 301 306-307 309 313 15-316 522-323 326-327 333-334 337 341 343-346 535 361 364 370 387 390-392 304 404 409 412415 421 428 430-432 469-342 300 312-313 339 382 427 444 404 409 412415 421 428 43 40-432 459-392 300 312-313 339 382 427 444 195 200 242 247 49 53 83 121 134 136 151 153 159 5202 128-219 223 247 244 247 246 267 269 302 312-313 339 382 427 444 195 200 242 247 40 247 49 53 83 121 134 136 151 153 161 161 161 161 161 161 161 161 161 16 | | | | 40 43 45 47 49-51 53-54 57-58 62 64 66 |
| 136 138-139 142-146 148 150-151 163 167 170-171 175 180 186-187 180 197 200 212 224 226-227 241 244 247-248 230-251 223-255 257-258 269 262-263 265 269 272 276-280 282-283 288 299 301 306-307 309 313 315-316 322-322 326-327 333-343 37 341 343-346 356 361 364 370 387 390-392 404 409 412 415 421 428 430-432 465 4-73 172 04 24 74 95 58 312 11 31 31 51 51 151 31 51 51 151 31 51 51 51 31 51 51 51 32 502 218-219 222 347 264 267 269 302 312-313 339 382 427 444 13 136 151 151 51 51 51 51 51 51 51 52 502 218-219 222 347 264 267 269 302 312-313 339 382 427 442 267 269 302 312-313 339 382 427 442 367 269 302 312-313 339 382 427 442 367 269 302 312-313 339 382 427 442 367 269 302 312-313 339 382 427 442 367 269 302 312-313 339 382 427 442 367 269 302 312-313 339 382 427 442 367 269 302 312-313 339 382 427 442 367 269 302 312-313 339 382 427 442 367 269 302 312-313 339 382 427 442 367 269 302 312-313 339 382 427 442 367 269 302 312-313 339 382 427 442 367 269 302 312-313 339 382 427 442 367 269 302 312-313 339 382 427 442 37 392 302 333 336 341 412 | | | | |
| 170-171 175 180 186-187 189 197 200 212 242 242 252 774 124 247 248 250-215 253-255 257-258 360 262-263 265 269 272 273 255-257-258 360 262-263 265 269 272 276-280 282-283 288 290 301 306-307 300 313 315-316 322-323 326-327 333-334 337 341 343-346 556 561 364 370 387 390-392 404 409 41 241 542 142 48 244 340-432 487-495 383 121 134 136 151 153 155 202 2182-139 223 247 264 267 269 302 312-313 339 382 427 444 242 262 277 244 27 49 53 83 121 134 136 151 153 155 202 218-219 223 247 264 267 269 302 312-313 339 382 427 444 222 242 277 240 247 264 267 269 302 312-313 339 382 427 444 222 281 396 427 472-473 247 24 27 24 247 264 267 269 302 312-313 339 382 427 444 222 281 396 427 472-473 247 24 27 24 27 24 247 247 | l | | | |
| 224 226-227 241 244 247-248 250-251 | | | i | |
| 233-255 257-258 260 262-263 265 269 272 276-280 282-283 288 209 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 306-307 301 301 301 301 301 301 301 301 301 301 | 1 | | ! | |
| 276-280 282-282 288 290 301 306-307 309 313 315-316 322-323 236-3273 33-343 341 343-346 356 361 364 370 387 390-392 404 409 412.415 421 428 42 484 340-432 459-473 induced neuron cells | | | | |
| Stratagene NTD001 | | | | |
| 341 343-346 356 361 364 370 387 390-392 | | | | |
| Moduced neuron Stratagene NTD001 7 20 42 44 49 5 38 312 113 43 16 15 11 31 31 15 15 11 31 31 5 15 11 31 31 5 15 11 31 31 5 15 11 31 31 5 15 11 31 31 31 5 15 11 31 31 31 5 15 11 31 31 31 5 15 11 31 31 31 5 15 11 31 31 31 5 15 11 31 31 31 5 15 11 31 31 31 5 15 11 31 31 31 5 15 12 31 31 31 31 31 31 31 31 31 31 31 31 31 | l . | Į. | | |
| Induced neuron cells | | | | |
| 195 202 218-219 223 247 264 267 269 302 | induced neuron | Stratagene | NTD001 | |
| Stratagene NTR001 34 70-72 104-106 110 116 197 258 392 396 induced neuronal cells Stratagene NTR001 34 70-72 104-106 110 116 197 258 392 396 422 422 422 423 | | Stratagene | 1112001 | |
| Stratagene NTR001 34 70-72 104-106 110 116 197 258 392 396 induced neuronal cells neuronal cells Stratagene NTU001 16 40 49 53-54 80 100 130 136 194 258 281 396 427 472-473 pituitary gland Clontech PIT004 54 119 170 200 242 264 270 319-320 333 336 341 414 placenta Clontech PLA003 32 390 341 421 prostate Clontech PRT001 78 180 182-183 187 209 250-251 273 278 292-393 306 329 333 336 409 442 rectum Invitrogen REC001 51 21 5 22 32 42 80 108 118 127 143-144 444 444 444 444 444 444 444 444 444 444 444 444 444 444 444 444 445 444 446 446 446 446 447 04 66 88 102 104-106 126 128 151 162 182 212 222 242 25 277 287 312 319-320 348 336 349 444 28 1819 43 24 26 577 288 345 396 640 442 444 448 449 | 001.5 | | | |
| Induced neuronal cells Stratagene NTU001 16 40 49 53-54 80 100 130 136 194 258 | retinoic acid- | Stratagene | NTR001 | |
| Colorect | | | | 422 |
| Reuronal cells Stratagene | | | ì | |
| Pituitary gland | | Stratagene | NTU001 | 16 40 49 53-54 80 100 130 136 194 258 |
| | | | | |
| Daleenta | pituitary gland | Clontech | PIT004 | 54 119 170 200 242 264 270 319-320 333 |
| PRT001 | | | } | 336 341 414 |
| 162 178 180 182-183 187 209 250-251 273 278 292-293 306 329 333 364 409 442 187 194 224 226 277 298 345 396 404 442 187 194 224 226 277 298 345 396 404 442 187 194 224 226 277 298 345 396 404 442 187 194 224 226 277 298 345 396 404 442 320 348 369 | placenta | Clontech | PLA003 | |
| TREQUESTION TRECORD | prostate | Clontech | PRT001 | |
| RECOUNT STATE ST | 1 | | | |
| 187 104 224 226 277 298 345 396 404 442 | | | | |
| 444 47 10 40 66 88 102 104 106 126 128 151 162 182 212 222 242 252 277 287 312 319-320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 348 369 320 320 348 369 320 | rectum | Invitrogen | REC001 | |
| Salivary gland Clontech SAL001 47 10 40 66 88 102 104-106 126 128 151 162 182 212 222 242 252 277 287 312 319-320 348 369 320 348 369 320 348 369 348 36 | | | | |
| 162 182 212 222 242 252 277 287 312 319- 320 348 369 320 348 369 42 | | | | |
| Salivary gland Clontech SALS03 42 | salivary gland | Clontech | SAL001 | |
| Salivary gland Sching Salivary gland Skin fibroblast ATCC SFB001 54 | | | | |
| Skin fibroblast ATCC SFB001 54 | 12 1 | CT | CA1 CO2 | |
| SKINDOI | | | | |
| Similar Simi | | | | |
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| thymus thyroid gland | Cloatech | THMc02 | 249 258-259 263-264 284 289 292 298 302 309 311 314 319-320 322-323 329 333 336 314 352 360 371 412 417 440 447 467 472-473 9-10 15 17 24-25 27-28 34 38 40 43 49 57-38 68 74 77 81 87 94-95 98 104-108 110 115-116 128 136-137 143 146 148-151 158 160 165 197 200 210-211 215 221-222 232 235 241 243 245 248 252 269 278 281 286 288-289 292 302 312 321 325 327 329 331 333 338 343 340 365 378 383 387 412 428 439-440 446 451-452 460 455 469-473 14-5 8-9 11-12 14-15 17 19 21-25 27 34 64 64 54 555-57-95 16-26 66-68 70-78 0-81 85 93 97-98 102-108 116 119 121-122 124 126-133 141-142 144 146 150-151 155 162-166 169 171 175-176 178-181 187-190 202-205 208 214-215 218-219 262 232 237-239 244 246-247 250-252 257-258 260 263-264 267 270-271 77 279 282-284 287-288 292 294 297 300 302-304 307-308 310-111 313 317 322-323 325 333 336-337 341 346 356 558 401 405-406 408-409 436 |
|----------------------|----------|--------|---|
| trachea | Clontech | TRC001 | 461 17 23 34 90 93 108 142 151 238 240 246 259 266 333 412 472-473 |
| uterus | Clontech | UTR001 | 18 20 30-31 50 52 114 125 158 164 168 182 198 206 210 248 254-255 260 273 283 304 311 325 365 383 421 423 |

The 16 tissue/mRNAs and their vendor sources are as follows: 1) Normal adult brain mRNA (Invitrogen), 2) Normal adult kidney mRNA (Invitrogen), 3) Normal fetal brain mRNA (Invitrogen), 4) Normal adult liver mRNA (Invitrogen), 5) Normal fetal kidney mRNA (Invitrogen), 6) Normal fetal liver mRNA (Invitrogen), 7) normal fetal kidney mRNA (Invitrogen), 8) human adrenal gland mRNA (Clontech), 9) Human bone marrow mRNA (Clontech), 10) Human leukemia lymphoblastic mRNA (Clontech), 11) Human thymus mRNA (Clontech), 12) human lymph node mRNA (Clontech), 13) human solspinal cord mRNA (Clontech), 14) human thyroid mRNA (Clontech), 15) human esophagus mRNA (BioChain), 16) human conceptional umbilical cord mRNA (BioChain).

TABLE 2

| SEQ ID | Accession | Species | Description | Score | % |
|--------|------------|------------------------------|--|-------|----------|
| NO: | No. | Species | Description | Score | Identity |
| 445 | gi4151328 | Homo sapiens | high-risk human papilloma viruses E6 oncoproteins targeted protein E6TP1 alpha mRNA, complete cds. | 2344 | 48 |
| 445 | gi4151330 | Homo sapiens | high-risk human papilloma viruses E6 oncoproteins targeted protein E6TP1 beta mRNA, complete cds. | 1694 | 59 |
| 445 | gi2555183 | Rattus norvegicus | SPA-1 like protein p1294 | 2324 | 48 |
| 446 | gi13517972 | Homo sapiens | PR-domain containing protein 17 mRNA, complete cds. | 2496 | 100 |
| 446 | gi10434545 | Homo sapiens | cDNA FLJ12827 fis, clone NT2RP2002939, weakly similar to ZINC FINGER PROTEIN 136. | 2496 | 100 |
| 446 | gi13623607 | Homo sapiens | , zinc finger protein 136 (clone pHZ-20), clone MGC:12711, mRNA, complete cds. | 710 | 42 |
| 447 | gi6093239 | Homo sapiens | mRNA; cDNA DKFZp434O0515 (from clone DKFZp434O0515). | 1054 | 100 |
| 447 | gi3522970 | Homo sapiens | Trio mRNA, complete cds. | 216 | 23 |
| 447 | AAW27227 | Homo sapiens | Human TRIO phosphoprotein. | 216 | 23 |
| 448 | gi7022890 | Homo sapiens | cDNA FLJ10700 fis, clone NT2RP3000665. | 2838 | 96 |
| 448 | gi10438668 | Homo sapiens | cDNA: FLJ22327 fis, clone HRC05572. | 1333 | 100 |
| 448 | gi7020045 | Homo sapiens | cDNA FLJ20140 fis, clone COL07182. | 1074 | 79 |
| 449 | gi6102903 | Homo sapiens | mRNA; cDNA DKFZp566D244 (from clone DKFZp566D244); partial cds. | 2601 | 99 |
| 449 | gi10434000 | Homo sapiens | cDNA FLJ12485 fis, clone NT2RM2000420. | 1907 | 100 |
| 449 | gi10437387 | Homo sapiens | cDNA: FLJ21308 fis, clone COL02131. | 1519 | 69 |
| 450 | gi7670836 | Homo sapiens | hepatocellular carcinoma-associated antigen 66 (HCA66) mRNA, complete cds. | 3101 | 99 |
| 450 | gi7959764 | Homo sapiens | PRO1289 | 935 | 100 |
| 450 | gi927708 | Saccharomyce s cerevisiae | Ydr449cp; CAI: 0.18 | 288 | 32 |
| 451 | gi7020902 | Homo sapiens | cDNA FLJ20657 fis, clone KAT01069. | 3231 | 99 |
| 451 | gil1037252 | Rattus norvegicus | NPL4 | 3156 | 96 |
| 451 | gi10434779 | Homo sapiens | cDNA FLJ12984 fis, clone NT2RP3000047, weakly similar to NPL4 PROTEIN. | 2812 | 99 |
| 452 | gi13160469 | Homo sapiens | WDR13 protein (WDR13) gene, complete cds. | 1063 | 94 |
| 452 | gi12044400 | Homo sapiens | WDR13 protein (WDR13) mRNA, complete cds. | 1063 | 94 |
| 452 | gi13751862 | Mus musculus | WD-repeat protein | 1058 | 93 |
| 453 | gi12619286 | Homo sapiens | mRNA for spinal cord-derived protein FI58G, complete cds. | 1133 | 100 |
| 453 | gi7638241 | Homo sapiens | mesenchymal stem cell protein DSC92 mRNA, complete cds. | 1133 | 100 |
| 453 | gi12804543 | Homo sapiens | , mesenchymal stem cell protein DSC92, clone MGC:2824, mRNA, complete cds. | 1133 | 100 |
| 454 | gi13279287 | Homo sapiens | , clone IMAGE:3633354, mRNA, partial cds. | 2066 | 100 |
| 454 | gi5052586 | Drosophila melanogaster | BcDNA.GH08385 | 334 | 25 |
| 454 | gi10433073 | Homo sapiens | cDNA FLJ11749 fis, clone | 190 | 26 |

| SEQ ID NO: | Accession No. | Species | Description . | Score | % Identity |
|---------------|------------------|----------------------------|--|-------|---------------|
| NO. | 110. | | HEMBA1005558, weakly similar to NUCLEAR PROTEIN SNF7. | | Identity |
| 455 | gi7019840 | Homo sapiens | cDNA FLJ20018 fis, clone ADSE00909. | 1698 | 99 |
| 455 | gi13938166 | Homo sapiens | , clone MGC:12617, mRNA, complete cds. | 1630 | 98 |
| 455 | gi9280376 | Homo sapiens | ancient conserved domain protein 3 (ACDP3) mRNA, complete cds. | 1271 | 90 |
| 456 | gi7020190 | Homo sapiens | cDNA FLJ20232 fis, clone COLF5593. | 1487 | 100 |
| 456 | gi14249896 | Homo sapiens | , clone MGC:15774, mRNA, complete cds. | 1479 | 99 |
| 456 | gi9188416 | Homo sapiens | Novel human gene mapping to chomosome 22. | 1479 | 99 |
| 457 | AAW75093 | Homo sapiens | Human secreted protein encoded by gene 37 clone HFVGS85. | 369 | 100 |
| 457 . | gi8895089 | Homo sapiens | protein x 013 mRNA, complete cds. | 145 | 41 |
| 457 | gi14250569 | Homo sapiens | , protein x 013, clone MGC:3073, mRNA, complete cds. | 145 | 41 |
| 458 | gi7020228 | Homo sapiens | cDNA FLJ20257 fis, clone COLF7231. | 1169 | 100 |
| 458 | gi7528184 | Drosophila melanogaster | bicoid-interacting protein BIN3 | 389 | 45 |
| 459 | gi11345384 | Homo sapiens | vacuolar protein sorting protein 18 (VPS18) mRNA, complete cds. | 5102 | 100 |
| 459 | AAW48303 | Homo sapiens | Amino acid sequence of human deep orange protein. | 2555 | 100 |
| 459 | gi2832850 | Drosophila melanogaster | EG:171E4.1 | 1316 | 35 |
| 460 | gi6966967 | Homo sapiens | mRNA for dipeptidyl-peptidase III (DPP3 gene). | 3814 | 99 |
| 460 | gi13938201 | Homo sapiens | , dipeptidylpeptidase III, cione MGC:15061, mRNA, complete cds. | 3811 | 99 |
| 460 | AAB67571 | Homo sapiens | Amino acid sequence of a human hydrolytic enzyme HYENZ3. | 3807 | 99 |
| 461 | AAY53020 | Homo sapiens | Human secreted protein clone qb56_19 protein sequence SEQ ID NO:46. | 657 | 100 |
| 461 | AAY59788 | Homo sapiens | Human normal ovarian tissue derived protein 65. | 618 | 100 |
| 461 | AAG04028 | Homo sapiens | Human secreted protein, SEQ ID NO: 8109. | 442 | 72 |
| 462 | gi13021843 | Homo sapiens | polyadenylate binding protein-interacting protein 2 mRNA, complete cds. | 679 | 100 |
| 462 | gi12052806 | Homo sapiens | mRNA; cDNA DKFZp564F163 (from clone DKFZp564F163); complete cds. | 675 | 99 |
| 462 | gi7106826 | Homo sapiens | HSPC218 | 673 | 99 |
| 463 | gi7023258 | Homo sapiens | cDNA FLJ10914 fis, clone OVARC1000212. | 1067 | 100 |
| 464 | gi7023258 | Homo sapiens | cDNA FLJ10914 fis, clone OVARC1000212. | 649 | 72 |
| 465 | gi7022147 | Homo sapiens | cDNA FLJ10233 fis, clone HEMBB1000266. | 3464 | 100 |
| 465 | gi12224837 | Homo sapiens | mRNA; cDNA DKFZp547K202 (from clone DKFZp547K202). | 3464 | 100 |
| 465 | AAY99662 | Homo sapiens | Human GTPase associated protein-13. | 3464 | 100 |
| 466 | gi7582304 | Homo sapiens | BM-016 | 584 | 100 |
| 466 | AAW85610 | Homo sapiens | Secreted protein clone eh80_1. | 330 | 97 |
| 466 | AAW78199 | Homo sapiens | Human secreted protein encoded by gene 74 clone HGBAC11. | 330 | 97 |
| 467 | gi7018410 | Homo sapiens | mRNA; cDNA DKFZp566K023 (from clone DKFZp566K023). | 1010 | 100 |
| 467 | gi9049987 | Rattus | X2CR1 protein | 268 | 81 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|---------------------------|---|--------------|---------------|
| 110. | 110. | norvegicus | | | Ruchtity |
| 468 | gi8317213 | Homo sapiens | histone acetyltransferase (MOF) mRNA, partial cds. | 1625 | 100 |
| 468 | gi10433157 | Homo sapiens | cDNA FLJ11810 fis, clone HEMBA1006347, moderately similar to MALES-ABSENT ON THE FIRST PROTEIN (EC 2.3.1). | 1625 | 100 |
| 468 | gi10436400 | Homo sapiens | cDNA FLJ14040 fis, clone HEMBA1005513, weakly similar to MALES-ABSENT ON THE FIRST PROTEIN (BC 2.3.1). | 1613 | 99 |
| 469 | AAY76072 | Homo sapiens | Human skin cell protein, SEQ ID NO:327. | 668 | 100 |
| 469 | AAB56011 | Homo sapiens | Skin cell protein, SEQ ID NO: 327. | 668 | 100 |
| 470 | gi29481 | Homo sapiens | Human erythrocyte 2,3- bisphosphoglycerate mutase mRNA EC 2.7.5.4. | 1362 | 100 |
| 470 | gi 179527 | Homo sapiens | Human 2,3-bisphosophoglycerate mutase (BPGM) gene, exon 3. | 1362 | 100 |
| 470 | AAB11959 | Homo sapiens | Glycated human erythrocyte bisphosphoglycerate mutase (BPGM). | .1362 | 100 |
| 471 | gi6841472 | Homo sapiens | HSPC125 | 892 . | 100 |
| 471 | gi12001966 | Homo sapiens | clone 015g09 My013 protein mRNA, complete cds. | 892 | 100 |
| 471 | gi9624483 | Homo sapiens | HRPAP20 short form mRNA, complete cds. | 640 | 72 |
| 472 | gi9367763 | Homo sapiens | mRNA for zinc finger protein Cezanne (CEZANNE gene). | 2580 | 100 |
| 472 | gi6102920 | Homo sapiens | mRNA; cDNA DKFZp434H0717 (from clone DKFZp434H0717); partial cds. | 2197 | 100 |
| 472 | gi7332054 | Caenorhabditis elegans | contains similarity to tumor necrosis factors | 126 | 25 |
| 473 | gi8489813 | Homo sapiens | DJ963K23.2 mRNA, complete cds. | 1255 | 100 |
| 473 | AAB43861 | Homo sapiens | Human cancer associated protein sequence SEQ ID NO:1306. | 1255 | 100 |
| 473 | gi9858803 | Mus musculus | Zfp228 | 1090 | 91 . |
| 474 | gi7020223 | Homo sapiens | cDNA FLJ20254 fis, clone COLF6926. | 2278 | 100 |
| 474 | AAY25743 | Homo sapiens | Human secreted protein encoded from gene 33. | 917 | 100 |
| 474 | AAY76166 | Homo sapiens | Human secreted protein encoded by gene 43. | 724 | 94 |
| 475 | gi14042066 | Homo sapiens | cDNA FLJ14503 fis, clone NT2RM1000252, weakly similar to H.sapiens E-MAP-115 mRNA. | 159 | 26 |
| 475 | gi7270600 | Arabidopsis thaliana | trichohyalin like protein | 156 | 25 . |
| 475 | gi180195 | Homo sapiens | Human aorta caldesmon mRNA, complete cds. | 145 | 25 |
| 476 | gi11066250 | Homo sapiens | presenilins associated rhomboid-like protein (PARL) mRNA, complete cds. | 2030 | 100 |
| 476 | gi13177766 | Homo sapiens | , Similar to presentiins associated rhomboid-like protein, clone MGC:4756, mRNA, complete cds. | 1107 | 99 |
| 476 | gi7959883 | Homo sapiens | PRO2207 | 986 | 100 |
| 477 | AAY91941 | Homo sapiens | Human chaperone protein 2 (HCHP-2). | 1977 | 100 |
| 477 | gi7019854 | Homo sapiens | cDNA FLJ20027 fis, clone ADSE01901. | 1965 | 99 |
| 477 | gi6567172 | Mus musculus | mDj10 | 1863 | 93 |
| 478 | gi13937971 | Homo sapiens | ; Similar to RIKEN cDNA 1110005A23 gene, clone MGC:14726, mRNA, | 1040 | 100 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|----------------------|---|-------|---------------|
| | | | complete cds. | | |
| 478 | gi13940310 | Homo sapiens | HCC-1 gene. | 1040 | 100 |
| 478 | AAB36609 | Homo sapiens | Human FLEXHT-31 protein sequence SEQ ID NO:31. | 1040 | 100 |
| 479 | gi11065999 | Homo sapiens | neuronal calcium binding protein NECAB3 mRNA, complete cds. | 1889 | 99 |
| 479 | gi10798741 | Homo sapiens | XB51 mRNA for X11L-binding protein 51, complete cds. | 654 | 99 |
| 479 | gi10798743 | Mus musculus | X11L binding protein 51 | 1079 | 86 |
| 480 | gi6094684 | Homo sapiens | PAC clone RP1-278D1 from X, complete sequence. | 3056 | 92 |
| 480 | gi10435614 | Homo sapiens | cDNA FLJ13568 fis, clone PLACE1008368, weakly similar to RING CANAL PROTEIN. | 1847 | 100 |
| 480 | gi7023516 | Homo sapiens | cDNA FLJ11078 fis, clone PLACE1005102, weakly similar.to RING CANAL PROTEIN. | 1208 | 42 |
| 481 | gi7020424 | Homo sapiens | cDNA FLJ20369 fis, clone HEP19364. | 2727 | 100 |
| 481 | gi1110599 | Mus sp. | semaphorin homolog=M-Sema F | 2653 | 86 |
| 481 | AAB88485 | Homo sapiens | Human membrane or secretory protein clone PSEC0078. | 1774 | 100 |
| 482 | gi4679028 | Homo sapiens | HSPC021 | 1930 | 100 |
| 482 | gi5106781 | Homo sapiens | HSPC025 | 1930 | 100 |
| 482 | gi12654535 | Homo sapiens | , HSPC025, clone MGC:735, mRNA, complete cds. | 1930 | 100 |
| 483 | gi1145789 | Rattus norvegicus | neuroligin 2 | 4417 | 98 |
| 483 | gi7960135 | Homo sapiens | neuroligin 3 isoform gene; complete cds, alternatively spliced. | 2736 | 65 |
| 483 | gi7960131 | Homo sapiens | neuroligin 3 isoform HNL3 mRNA, complete cds, alternatively spliced. | 2729 | 65 |
| 484 | gi14250554 | Homo sapiens | , hexokinase 1, clone MGC:1724, mRNA, complete cds. | 4725 | 99 |
| 484 | gi2873349 | Homo sapiens | hexokinase I (HK1) gene, exon 18, complete cds, alternatively spliced. | 4725 | 99 |
| 484 | gi184021 | Homo sapiens | Human hexokinase 1 (HK1) mRNA, complete cds. | 4718 | 99 |
| 485 | gi8453103 | Homo sapiens | zinc finger protein mRNA, complete cds. | 3726 | 100 |
| 485 | gi13752754 | Homo sapiens | zinc finger 1111 mRNA, complete cds. | 1689 | 56 |
| 485 | gi10436789 | Homo sapiens | cDNA FLJ14345 fis, clone THYRO1001189, weakly similar to ZINC FINGER PROTEIN 91. | 1683 | 56 |
| 486 | AAB56937 | Homo sapiens | Human prostate cancer antigen protein sequence SEQ ID NO:1515. | 2341 | 100 |
| 486 | gi12804453 | Homo sapiens | , Similar to Tu translation elongation factor, mitochondrial, clone MGC:1592, mRNA, complete cds. | 2326 | 100 |
| 486 | gi899285 | Homo sapiens | H.sapiens mRNA for elongations factor Tu-mitochondrial. | 2326 | 100 |
| 487 | gi9910111 | Homo sapiens | myosin X (MYO10) mRNA, complete cds. | 10727 | 99 |
| 487 | gi6996558 | Mus musculus | myosin X | 10089 | 93 |
| 487 | gi7108753 | Homo sapiens | myosin X (MYO10) mRNA, partial cds. | 8029 | 99 |
| 488 | gi7688687 | Homo sapiens | AD-017 protein mRNA, complete cds. | 1935 | 100 |
| 488 | gi14042251 | Homo sapiens | cDNA FLJ14611 fis, clone NT2RP1000988. | 1935 | 100 |
| | AAY66671 | Homo sapiens | Membrane-bound protein PRO1134. | 1935 | 100 |
| 488 489 | gi202215 | Mus musculus | alpha-tubulin isotype M-alpha-6 | 2387 | 100 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|----------------------------|--|-------|---------------|
| | | | mRNA, complete cds. | | |
| 489 | gi1333692 | Macaca fascicularis | alpha-tubulin (ATG-initiation codon missing) | 2382 | 100 |
| 490 | gi5912034 . | Homo sapiens | mRNA; cDNA DKFZp434N0535 (from clone DKFZp434N0535); partial cds. | 6810 | 99 |
| 490 | gi5912239 | Homo sapiens | mRNA; cDNA DKFZp434O225 (from clone DKFZp434O225); partial cds. | 3442 | 99 |
| 490 | gi3292939 | Drosophila melanogaster | Additional sex combs | 295 | 39 |
| 491 | gi5912034 | Homo sapiens | mRNA; cDNA DKFZp434N0535 (from clone DKFZp434N0535); partial cds. | 5941 | 99 |
| 491 | gi5912239 | Homo sapiens | mRNA; cDNA DKFZp434O225 (from clone DKFZp434O225); partial cds. | 2573 | 99 |
| 491 | gi3292939 | Drosophila melanogaster | Additional sex combs | 295 | 39 |
| 492 | AAY68778 | Homo sapiens | Amino acid sequence of a human phosphorylation effector PHSP-10. | 2463 | 99 |
| 492 | gi479173 | Homo sapiens | H.sapiens nek3 mRNA for protein kinase. | 2417 | 99 |
| 492 | gi13529320 | Mus musculus | Similar to NIMA (never in mitosis gene a)-related expressed kinase 3 | 1887 | 73 |
| 493 | gi13539686 | Homo sapiens | protein kinase C and casein kinase substrate I (PACSINI) mRNA, complete cds. | 2365 | 100 |
| 493 | gi728604 | Mus musculus | PACSIN | 2250 | .95 |
| 493 | gi4324452 | Rattus | syndapin I | 2250 | 95 |
| 494 | gi7023749 | Homo sapiens | cDNA FLJ11220 fis, clone PLACE1008129. | 3994 | 100 |
| 494 | gi10433501 | Homo sapiens | cDNA FLJ12104 fis, clone HEMBB1002697. | 2829 | 100 |
| 494 | gi5788108 | Homo sapiens | PAC clone RP5-1087M19 from 7q11.23- q21.1, complete sequence. | 757 | 63 |
| 495 | AAB54375 | Homo sapiens | Human pancreatic cancer antigen protein sequence SEQ ID NO:827. | 2897 | 99 |
| 495 | AAY57923 | Homo sapiens | Human transmembrane protein HTMPN- 47. | 2724 | 98 |
| 495 | AAW88628 | Homo sapiens | Secreted protein encoded by gene 95 clone HPWAN23. | 2686 | 98 |
| 496 | gi7959788 | Homo sapiens | PRO1635 | 317 | 100 |
| 496 | AAW74852 | Homo sapiens | Human secreted protein encoded by gene 124 clone HPCAD23. | 143 | 100 |
| 497 | gi7707424 | Homo sapiens | mRNA for syntaxin 18, complete cds. | 1705 | 100 |
| 498 | gi1613858 | Homo sapiens | Human zinc finger protein zfp47 (zf47) mRNA, partial cds. | 1488 | 83 |
| 498 | gi13938633 | Mus musculus | RIKEN cDNA 2810435N07 gene | 1318 | 60 |
| 498 | gi9837564 | Mus musculus | SCAN-KRAB-zinc finger protein | 1242 | 58 |
| 499 | AAY27795 | Homo sapiens | Human secreted protein encoded by gene No. 79. | 1539 | 99 |
| 499 | gi10436317 | Homo sapiens | cDNA FLJ13986 fis, clone Y79AA1001923, weakly similar to Homo sapiens F-box protein Fbx22 (FBX22) gene. | 1370 | 100 |
| 499 | gi6164747 | Homo sapiens | F-box protein Fbx22 (FBX22) gene, partial cds. | 391 | 93 |
| 500 | gi3150052 | Homo sapiens | TGF beta receptor associated protein-1 mRNA, complete cds. | 4455 | 100 |
| 500 | gi14280050 | Homo sapiens | Vps39/Vam6-like protein gene, complete cds. | 382 | 24 |
| 500 | gi12718237 | Neurospora | related to TGF beta receptor associated | 174 | 31 |

| SEQ ID | Accession | Species | Description | Score | % |
|--------|------------|------------------|--|-------|----------|
| NO: | No. | | | | Identity |
| | <u> </u> | crassa | protein 1 | | |
| 501 | gi7023051 | Homo sapiens | cDNA FLJ10796 fis, clone | 3360 | 99 |
| | 1 | | NT2RP4000648, weakly similar to TRANS-ACTING TRANSCRIPTIONAL | | |
| | | | PROTEIN ICPO. | | |
| 501 | gi9651170 | Homo sapiens | cell cycle checkpoint protein CHFR | 2491 | 96 |
| | 3 | | mRNA, complete cds. | | ' ' |
| 501 | AAB20219 | Homo sapiens | Human Chfr (checkpoint with FHA and | 2491 | 96 |
| | | | ring finger) protein. | | |
| 502 | gi7329074 | Homo sapiens | collagen type V alpha 3 chain (COL5A3) | 9671 | 100 |
| 502 | -:0560004 | Rattus | mRNA, complete cds. alpha 4 type V collagen | 8038 | 82 |
| 302 | gi8568094 | norvegicus | aipna 4 type v conagen | 0030 | 82 |
| 502 | gi7329072 | Mus musculus | collagen type V alpha 3 chain | 7970 | 82 |
| 503 | gi12654687 | Homo sapiens | , clone MGC:2616, mRNA, complete cds. | 1161 | 100 |
| 503 | gi7769617 | Mus musculus | TCE2 | 1050 | 89 |
| 504 | gi12654687 | Homo sapiens | , clone MGC:2616, mRNA, complete cds. | 1140 | 96 |
| 504 | gi7769617 | Mus musculus | TCE2 | 1029 | 86 |
| 505 | gi12654687 | Homo sapiens | , clone MGC:2616, mRNA, complete cds. | 654 | 100 |
| 505 | gi7769617 | Mus musculus | TCE2 | 629 | 92 |
| 506 | gi14249942 | Homo sapiens | , Similar to RIKEN cDNA 0610008P16 | 1609 | 100 |
| | | | gene, clone MGC:15937, mRNA, | | |
| 506 | AAB56487 | Homo sapiens | complete cds. Human prostate cancer antigen protein | 1167 | 98 |
| 300 | AAB36487 | Homo sapiens | sequence SEQ ID NO:1065. | 1107 | 98 |
| 506 | gi2828262 | Bos taurus | aralkyl acyl-CoA;amino acid N- | 597 | 40 |
| | 3 | | acyltransferase | | 1 " |
| 507 | gi7688987 | Homo sapiens | uncharacterized bone marrow protein | 1295 | 100 |
| | | | BM046 | | |
| 507 | AAB64387 | Home sapiens | Amino acid sequence of human | 1202 | 94 |
| | | | intracellular signalling molecule | | i |
| 507 | gi9437511 | Homo sapiens | INTRA19. BM024 | 1045 | 98 |
| 508 | AAB18979 | Homo sapiens | Amino acid sequence of a human | 1203 | 100 |
| 308 | AAD 10313 | 110illo sapiciis | transmembrane protein. | 1203 | 1.00 |
| 508 | gi6808196 | Homo sapiens | mRNA; cDNA DKFZp434P1018 (from | 938 | 100 |
| | | | clone DKFZp434P1018); partial cds. | | |
| 508 | gi13960126 | Homo sapiens | , Similar to leucine-rich neuronal protein, | 845 | 100 |
| | L | <u> </u> | clone MGC:4126, mRNA, complete cds. | | · |
| 509 | gi13938527 | Homo sapiens | , Similar to RIKEN cDNA 2810002N01 | 1048 | 100 |
| | 1 | | gene, clone MGC:2562, mRNA, complete cds. | | |
| 509 | AAY35994 | Homo sapiens | Extended human secreted protein | 1032 | 98 |
| 507 | 711133354 | Tionio sapiens | sequence, SEQ ID NO. 379. | 1032 | 70 |
| 509 | AAG00345 | 'Homo sapiens | Human secreted protein, SEQ ID NO: | 619 | 98 |
| | | | 4426. | | |
| 510 | gi773387 | Neurospora | Restriction enzyme inactivation of met-10 | 536 | 35 |
| | | crassa | complementation in this region. Sequence | | |
| | | | similarity to S. cerevisiae chromosome VIII cosmid 9205, accession no. U10556 | i | |
| | | | CDS residues 22627-24126 | | |
| 510 | gi487945 | Saccharomyce | Yhr070wp | 528 | 49 |
| 5.0 | B.107313 | s cerevisiae | | 320 | ." |
| 510 | AAG02508 | Homo sapiens | Human secreted protein, SEQ ID NO: | 324 | 100 |
| | | | 6589. | | |
| 511 | gi11493195 | Homo sapiens | mRNA for LB1 protein. | 2614 | 99 |
| 511 | gi10434688 | Homo sapiens | cDNA FLJ12920 fis, clone | 2604 | 99 |
| 511 | gi12053201 | YYama samig | NT2RP2004594. | 2604 | 99 |
| 211 | B112033201 | Homo sapiens | mRNA; cDNA DKFZp434A1031 (from | 2004 | 77 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|----------------------------|--|-------|---------------|
| | | | clone DKFZp434A1031); complete cds. | | |
| 512 | AAW75106 | Homo sapiens | Human secreted protein encoded by gene 50 clone HHSDZ57. | 471 | 100 . |
| 512 | AAY59689 | Homo sapiens | Secreted protein 26-44-1-B5-CL3_1. | 471 | 100 |
| 512 | AAY48331 | Homo sapiens | Human prostate cancer-associated protein 28. | 471 | 100 |
| 514 | AAW67888 | Homo sapiens | Human secreted protein encoded by gene 82 clone HSKHL65. | 921 | 92 |
| 514 | gi13436110 | Homo sapiens | , Similar to RIKEN cDNA 2310034L04 gene, clone MGC:11061, mRNA, complete cds. | 150 | 28 |
| 514 | AAY53052 | Homo sapiens | Human secreted protein clone df202_3 protein sequence SEQ ID NO:110. | 132 | 33 |
| 515 | gi7020259 | Homo sapiens | cDNA FLJ20276 fis, clone HEP02437. | 5378 | 100 |
| 515 | gi10432807 | Homo sapiens | cDNA FLJ11534 fis, clone HEMBA1002679. | 3024 | 99 |
| 515 | gi9916 | Plasmodium falciparum | liver stage antigen | 399 | 23 |
| 516 | AAB67448 | Homo sapiens | Amino acid sequence of a human chaperone polypeptide. | 1190 | 99 |
| 516 | gi13477189 | Homo sapiens | , Similar to RIKEN cDNA 1300007M11 gene, clone MGC:12943, mRNA, complete cds. | 1182 | 99 |
| 516 | AAG03527 | Homo sapiens | Human secreted protein, SEQ ID NO: 7608. | 389 | 98 |
| 517 | gi7023782 | Homo sapiens | cDNA FLJ11240 fis, clone PLACE1008568. | 2796 | 100 |
| 517 | AAB08869 | Homo sapiens | Amino acid sequence of a human secretory protein. | 2792 | 99 |
| 517. | AAB23626 | Homo sapiens | Human secreted protein SEQ ID NO: 52. | 2792 | 99 |
| 518 | gi6460009 | Deinococcus radiodurans | citrate lyase, beta subunit | 211 | 30 |
| 518 | gi14025765 | Mesorhizobiu m loti | citrate lyase beta-subunit | 324 | 31 |
| 518 | gi14024477 | Mesorhizobiu m loti | Citrate lyase beta chain (acyl lyase subunit); CitE | 316 | 33 |
| 519 | gi14041831 | Homo sapiens | cDNA FLJ14357 fis, clone HEMBA1000005, highly similar to DNAJ PROTEIN HOMOLOG MTJ1. | 2873 | 100 |
| 519 | AAB67447 | Homo sapiens | Amino acid sequence of a human chaperone polypeptide. | 2481 | 99 |
| 519 | gi473847 | Mus musculus | dnaJ-like protein | 2413 | 84 |
| 520 | gi7669968 | Homo sapiens | mRNA; cDNA DKFZp761G0313 (from clone DKFZp761G0313). | 789 | 100 |
| 520 | gi4586315 | Homo sapiens | ORCTL3 mRNA for organic-cation transporter like 3, complete cds. | 348 | 38 |
| 520 | gi4835384 | Homo sapiens | DNA, DLEC1 to ORCTL4 gene region, section 1/2 (DLEC1, ORCTL3, ORCTL4 genes, complete cds). | 348 | 38 |
| 521 | gi7959805 | Homo sapiens | PRO0823 | 344 | 100 |
| 522 | gi10434341 | Homo sapiens | cDNA FLJ12691 fis, clone NT2RM4002571, weakly similar to H.sapiens mRNA for UDP- GalNAc:polypeptide N- acetylgalactosaminyltransferase (T2). | 2605 | 89 |
| 522 | gi10436305 | Homo sapiens | cDNA FLJ13977 fis, clone Y79AA1001603, weakly similar to POLYPEPTIDE N- ACETYLGALACTOSAMINYLTRANS FERASE (EC 2.4.1.41). | 1631 | 99 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|------------------------------|---|-------|---------------|
| 522 | gi971461 | Homo sapiens | H.sapiens mRNA for UDP- GalNAc:polypeptide N- acetylgalactosaminyltransferase (T2). | 1386 | 50 |
| 523 | gi11493500 | Homo sapiens | PRO2979 | 477 | 100 |
| 523 | gi38163 | Pan | A-gamma-globin | 477 | 100 |
| | 8,501-0 | troglodytes | 1 - 9 | | |
| 523 | gi176779 | Pan troglodytes | gamma-2 globin | 477 | 100 |
| 524 | gi5262582 | Homo sapiens | mRNA; cDNA DKFZp434K063 (from clone DKFZp434K063); partial cds. | 3782 | 99 |
| 524 | gi10438230 | Homo sapiens | cDNA: FLJ21993 fis, clone HEP06576. | 1416 | 100 |
| 524 | AAY21842 | Homo sapiens | Human signal peptide-contianing protein (SIGP) (clone ID 1273453). | 1416 | 100 |
| 525 | gi1928886 | Rattus norvegicus | lin-10 protein homolog | 2199 | 97 |
| 525 | gi10433467 | Homo sapiens | cDNA FLJ12076 fis, clone HEMBB 1002442, weakly similar to LIN- 10 PROTEIN. | 483 | 98 |
| 525 | gi5824587 | Caenorhabditis elegans | T01G9.2b | 668 | 37 |
| 526 | gi1679607 | Mus musculus | myosin-I | 4206 | 84 |
| 526 | gi1924940 | Homo sapiens | H.sapiens mRNA for myosin-IE. | 4115 | 99 |
| 526 | gi65324 | Gallus gallus | brush border myosin IB | 3812 | 76 |
| 527 | AAB63419 | Homo sapiens | Human breast cancer associated antigen protein sequence SEQ ID NO:781. | 641 | 99 |
| 528 | gi13649967 | Homo sapiens | fovea-associated SH3 domain binding protein (FASH3) mRNA, complete cds. | 558 | .100 |
| 528 | gi13539561 | Homo sapiens | mRNA for SH3BGRL2 protein. | 558 | 100 |
| 528 | gi5042302 | Mus musculus | sh3bgr protein | 365 | 64 |
| 529 | gi10436540 | Homo sapiens | cDNA FLJ14154 fis, clone NT2RM1000341. | 1151 | 99 |
| 529 | gi13436011 | Mus musculus | RIKEN cDNA 1200013P24 gene | 1139 | 97 |
| 529 | gi1592161 | Methanococcu s jannaschii | ribosomal protein S18 alanine acetyltransferase | 109 | 36 |
| 530 | gi3135314 | Homo sapiens | chromosome 7q22 sequence, complete sequence. | 911 | 100 |
| 530 | gi6752287 | Homo sapiens | Novel human gene mapping to chomosome X. | 281 | 51 |
| 531 | gi14042818 | Homo sapiens | cDNA FLJ14937 fis, clone PLACE1010231, weakly similar to CELL SURFACE GLYCOPROTEIN EMRI PRECURSOR. | 2548 | 97 |
| 531 | gi2117161 | Homo sapiens | H.sapiens mRNA for HE6 Tm7 receptor. | 1366 | 52 |
| 531 | AAW36903 | Homo sapiens | Human epididymis-specific receptor protein. | 1366 | 52 |
| 532 | gi7417372 | Homo sapiens | intracellular hyaluronan-binding protein mRNA, complete cds. | 2175 | 99 |
| 532 | gi7110497 | Mus musculus | intracellular hyaluronan-binding protein p57 | 1862 | 85 |
| 532 | gi3403154 | Homo sapiens | Human Ki-1/57 intracellular antigen mRNA, partial cds. | 1591 | 98 |
| 533 | gì10436645 | Homo sapiens | cDNA FLJ14235 fis, clone NT2RP4000167. | 1585 | 82 |
| 533 | gi7020976 | Homo sapiens | cDNA FLJ20707 fis, clone KAJA1223. | 2195 | 84 |
| 533 | gi13276619 | Homo sapiens | mRNA; cDNA DKFZp761I0112 (from clone DKFZp761I0112). | 1444 | 99 |
| 534 | gi438880 | Rattus norvegicus | tropomyosin | 1186 | 99 |
| 534 | gi2978558 | Xenopus | alpha-tropomyosin | 1089 | 89 |
| | | | | | |

| SEO ID | Accession | Species | Description | Score | 1 % |
|--------|-------------|-------------------------------|---|-------|----------|
| NO: | No. | Opened | 2 Company | | Identity |
| | | laevis | | | |
| 534 | gi438882 | Rattus norvegicus | tropomyosin | 1086 | 92 |
| 535 | gi438880 | Rattus norvegicus | tropomyosin | 1120 | 93 |
| 535 | gi9508585 | Homo sapiens | tropomyosin isoform mRNA, complete cds. | 1105 | 93 |
| 535 | gi12653955 | Homo sapiens | , Similar to tropomyosin 4, clone MGC:3261, mRNA, complete cds. | 1094 | 91 |
| 536 | gi6808111 | Homo sapiens | mRNA; cDNA DKFZp434O1230 (from clone DKFZp434O1230); partial cds. | 439 | 100 |
| 537 | gi6807806 | Homo sapiens | mRNA; cDNA DKFZp434K031 (from clone DKFZp434K031); partial cds. | 3007 | 100 |
| 537 | gi13623334 | Homo sapiens | , Similar to DKFZP727C091 protein, clone MGC:10677, mRNA, complete cds. | 2392 | 100 |
| 537 | AAY25821 | Homo sapiens | Human secreted protein fragment encoded from gene 41. | 1967 | 99 . |
| 538 | AAB88413 | Homo sapiens | Human membrane or secretory protein clone PSEC0170. | 1818 | 99 |
| 538 | gi6457342 | Homo sapiens | E2IG4 (E2IG4) mRNA, complete cds. | 1813 | 99 |
| 538 | AAB24026 | Homo sapiens | Human PRO1788 protein sequence SEQ IDNO:18. | 1813 | 99 |
| 539 | gi6572289 | Homo sapiens | mRNA for mitochondrial tryptophanyl- tRNA synthetase (WARS2 gene). | 1820 | 100 |
| 539 | gi13421159 | Caulobacter crescentus | tryptophanyl-tRNA synthetase | 727 | 46 |
| 539 | gi11992026 | Zymomonas mobilis | tryptophanyl-tRNA synthase | 721 | 43 |
| 540 | gi7106630 | Homo sapiens | Novel human mRNA from chromosome I, clone Z98884, has homology to PERIOD CIRCADIAN PROTEIN 3. | 6301 | 99 |
| 540 | gi13160925 | Homo sapiens | mRNA for period (Drosophila) homolog 3 hPER3, complete cds. | 6274 | 99 |
| 540 | AAB23266 | Homo sapiens | Human circadian rhythm protein Per3 (hPer3). | 6274 | 99 |
| 541 | gi9621744 | Homo sapiens | ferritin heavy chain subunit mRNA, complete cds. | 968 | 100 |
| 541 | gi 12654093 | Homo sapiens | , ferritin, heavy polypeptide 1, clone MGC:5580, mRNA, complete cds. | 968 | 100 |
| 541 | gi12655095 | Homo sapiens | , ferritin, heavy polypeptide 1, clone MGC:1749, mRNA, complete cds. | 968 | 100 |
| 542 | gi4902699 | Homo sapiens | Novel human gene mapping to chomosome 13. | 2372 | 57 |
| 542 | gi2341020 | Homo sapiens | PAC clone 248O15 from 13q12-q13, complete sequence. | 1447 | 58 |
| 542 | gi11907986 | Drosophila melanogaster | fry | 1054 | 38 |
| 543 | gi7582278 | Homo sapiens | BM-003 | 1386 | 100 |
| 543 | gi7688983 | Homo sapiens | uncharacterized bone marrow protein BM044 | 1386 | 100 |
| 543 | gi1752736 | Saccharomyce s cerevisiae | gene required for phosphoylation of oligosaccharides/ has high homology with YJR061w | 150 | 35 |
| 544 | gi1628401 | Homo sapiens | H.sapiens mRNA for leucine-rich primary response protein 1. | 3936 | 98 |
| 544 | gi940821 | Rattus norvegicus | LRPRI | 2914 | 73 |
| 544 | gi2196560 | Schizosacchar omyces pombe | Mis6 | 223 | 31 |

| SEQ ID | Accession | Species | Description | Score | % Identity |
|--------|------------------|------------------------------|---|-------|---------------|
| NO: | No. gi7022824 | Homo sapiens | cDNA FLJ10656 fis, clone | 1574 | 99 |
| 545 | gi6841138 | Homo sapiens | NT2RP2006038. HSPC099 mRNA, partial cds. | 248 | 36 |
| 545 | AAG02788 | Homo sapiens | Human secreted protein, SEQ ID NO: | 234 | 85 |
| 546 | AAB71914 | Homo sapiens | Human ISOM-6. | 1142 | 98 |
| 546 | gi3876969 | Caenorhabditis elegans | Similarity to Brugia peptidylprolyl isomerase (TR-G98452), contains similarity to Pfam domain: PF00076 (RNA recognition motif. (a.k.a. RRM, RBD, or RNP domain); Score=62.0, E-value=4.2e-15, N=1; PF00160 (Cyclophilin type peptidyl-prolyl cis-trans isomerase), Score=78.1, E-value=3.7e-22, N=1 | 658 | 52 |
| 546 | AAG02246 | Homo sapiens | Human secreted protein, SEQ ID NO: 6327. | 573 | 100 |
| 547 | gi603635 | Saccharomyce s cerevisiae | Yel044wp | 133 | 25 |
| 548 | gi5262665 | Homo sapiens | mRNA; cDNA DKFZp564B0769 (from clone DKFZp564B0769); partial cds. | 1455 | 99 |
| 548 | gi6841172 | Homo sapiens | HSPC261 | 716 | 99 |
| 548 | gi12803875 | Homo sapiens | , Similar to splicing factor, arginine/scrine-rich 4, clone MGC:3920, mRNA, complete cds. | 352 | 33 |
| 549 | gi7582298 | Homo sapiens | BM-013 | 704 | 100 |
| 549 | gi9558483 | Ciona savignyi | PEM-3 | 434 | 55 |
| 549 | gi1644450 | Caenorhabditis elegans | MEX-3 | 362 | 65 |
| 550 | gi4883433 | Homo sapiens | mRNA for membrane transport protein (XK gene). | 2148 | 100 |
| 550 | gi6502963 | Mus musculus | KX antigen | 1797 | 81 |
| 550 | gi2580580 | Homo sapiens | testis-specific XK Related Y (XKRY) mRNA, complete cds. | 157 | 31 |
| 551 | gi7670746 | Homo sapiens | UDP-glucose:glycoprotein glucosyltransferase 1 precursor, mRNA, complete cds. | 8075 | 99 |
| 551 | gi13275621 | synthetic construct | Rat RUGT | 7371 | 91 |
| 551 | gi7677176 | Rattus norvegicus | UDP-glucose glycoprotein:glucosyltransferase precursor | 7371 | 91 |
| 552 | gi7688985 | Homo sapiens | uncharacterized bone marrow protein BM045 | 390 | 72 |
| 553 | gi12655091 | Homo sapiens | , AD-003 protein, clone MGC:783, mRNA, complete cds. | 1177 | 100 |
| 553 | gi6523799 | Homo sapiens | adrenal gland protein AD-003 mRNA, complete cds. | 1168 | 99 |
| 553 | gi7105659 | Caenorhabditis elegans | contains similarity to Streptomyces peucetius carminomycin 4-O- methyltransferase (GB:L13453) | 425 | 39 |
| 554 | gi7582282 | Homo sapiens | BM-005 | 3445 | 99 |
| 554 | gi7022933 | Homo sapiens | cDNA FLJ10725 fis, clone NT2RP3001214. | 3312 | 100 |
| 554 | gi10435575 | Homo sapiens | cDNA FLJ13534 fis, clone PLACE1006445. | 1648 | 100 |
| 555 | gi12751374 | Homo sapiens | paraoxanase-3 mRNA, partial cds. | 1819 | 99 . ' |
| 555 | gi1333634 | Homo sapiens | paraoxonase 3 (PON3) mRNA, 3' end of cds. | 1741 | 98 |
| 555 | gi12743899 | Oryctolagus | paraoxonase 3 | 1542 | 82 |

| SEQ ID | Accession | Species | Description | Score | % |
|--------|-------------|------------------------------|--|-------|-----------|
| NO: | No. | Species | Description | Beore | Identity |
| 110. | 110. | cuniculus | | | racintity |
| 556 | gi7022174 | Homo sapiens | cDNA FLJ10252 fis, clone HEMBB1000807. | 2826 | 100 |
| 556 | gil1596985 | Homo sapiens | chromosome 14 clone RP11-361H10 map 14q24.3, complete sequence. | 559 | 36 |
| 556 | gi7020945 | Homo sapiens | cDNA FLJ20689 fis, clone KAIA2890. | 510 | 39 |
| 557 | gi10434683 | Homo sapiens | cDNA FLJ12917 fis, clone NT2RP2004568, weakly similar to PUTATIVE ATP-DEPENDENT RNA HELICASE C30D11.03. | 2879 | 99 |
| 557 | gi13384106 | Homo sapiens | RNA helicase-like protein (RHLP) mRNA, complete cds. | 2817 | 99 |
| 557 | gi7020811 | Homo sapiens | cDNA FLJ20596 fis, clone KAT08049. | 2020 | 99 |
| 558 | gi4760710 | Brassica rapa | SLL2-S9-protein | 284 | 43 |
| 558 | gi1669601 | Arabidopsis thaliana | AR401 | 280 | 44 |
| 558 | gi557805 | Saccharomyce s cerevisiae | orf, len: 257, CAI: 0.13 | 327 | 34 |
| 559 | gi13548677 | Homo sapiens | MKP-7 mRNA for MAPK phosphatase-7, complete cds. | 3418 | 100 |
| 559 | gi13990989 | Mus musculus | MAP kinase phosphatase-7 | 3093 | 90 |
| 559 | AAB20325 | Homo sapiens | Human protein phosphatase and kinase protein-4. | 3021 | 90 |
| 560 | gi10433965 | Homo sapiens | cDNA FLJ12464 fis, clone NT2RM1000780. | 2196 | 97 |
| 560 | gi10434795 | Homo sapiens | cDNA FLJ12992 fis, clone NT2RP3000149. | 2196 | 97 |
| 560 | gi10438048 | Homo sapiens | cDNA: FLJ21857 fis, clone HEP02294. | 2151 | 94 |
| 561 | gi10438048 | Homo sapiens | cDNA: FLJ21857 fis, clone HEP02294. | 2276 | 97 |
| 561 | gi10433965 | Homo sapiens | cDNA FLJ12464 fis, clone NT2RM1000780. | 2159 | 94 |
| 561 | gi10434795 | Homo sapiens | cDNA FLJ12992 fis, clone NT2RP3000149. | 2159 | 94 |
| 562 | gi10433965 | Homo sapiens | cDNA FLJ12464 fis, clone NT2RM1000780. | 2443 | 99 |
| 562 | gi10434795 | Homo sapiens | cDNA FLJ12992 fis, clone NT2RP3000149. | 2443 | 99 |
| 562 | gi10438048 | Homo sapiens | cDNA: FLJ21857 fis, clone HEP02294. | 2398 | 96 |
| 563 | gi11137965 | Homo sapiens | tRNA isopentenylpyrophosphate transferase precursor RNA, complete cds. | 2158 | 100 |
| 563 | gi7019915 | Homo sapiens | cDNA FLJ20061 fis, clone COL01383. | 1719 | 100 |
| 563 | gi9803035 | Caenorhabditis elegans | contains similarity to Pfam domain PF00096 (zf-C2H2), Score=12.0, E- value=1.1, N=1 | 407 | 32 |
| 564 | gi7023103 | Homo sapiens | cDNA FLJ10826 fis, clone NT2RP4001100. | 2171 | 100 |
| 564 | gi10434339 | Homo sapiens | cDNA FLJ12690 fis, clone NT2RM4002567. | 2171 | 100 |
| 564 | gi10433458 | Homo sapiens | cDNA FLJ12068 fis, clone HEMBB1002329. | 2166 | 99 |
| 565 | gi7019829 | Homo sapiens | cDNA FLJ20011 fis, clone ADKA03432. | 865 | 100 |
| 565 | gi10438448. | Homo sapiens | cDNA: FLJ22168 fis, clone HRC00618. | 865 | 100 |
| 565 | AAG02581 | Homo sapiens | Human secreted protein, SEQ ID NO: 6662. | 445 | 98 |
| 566 | gi11558482 | Homo sapiens | mRNA for B-cell lymphoma/leukaemia 11A extra long form (BCL11A-XL gene). | 1543 | 99 |
| 566 | gi12150278 | Homo sapiens | C2H2-type zinc-finger protein mRNA, complete cds. | 1039 | 99 . |
| 566 | gi6652688 | Mus musculus | C2H2-type zinc finger protein | 1033 | 98 |

| SEQ ID | Accession | Species | Description | Score | % |
|--------|-------------|----------------------|---|--------|----------|
| NO: | No. | | PALL PALL DIGITAL COLLEGE CO. | | Identity |
| 567 | gi12053249 | Homo sapiens | mRNA; cDNA DKFZp434A155 (from clone DKFZp434A155); complete cds. | 994 | 100 |
| 567 | AAY73435 | Homo sapiens | Human secreted protein clone yd73_1 protein sequence SEQ ID NO:92. | 994 | 100 |
| 567 | AAB43698 | Homo sapiens | Human cancer associated protein sequence SEQ ID NO:1143. | 752 | 95 |
| 568 | gi12053249 | Homo sapiens | mRNA; cDNA DKFZp434A155 (from clone DKFZp434A155); complete cds. | 752 | 95 |
| 568 | AAY73435 | Homo sapiens | Human secreted protein clone yd73_1 protein sequence SEQ 1D NO:92. | 752 | 95 |
| 568 | AAB43698 | Homo sapiens | Human cancer associated protein sequence SEQ ID NO:1143. | 853 | 100 |
| 569 | gi8096260 | Homo sapiens | gene for Nop10p, complete cds. | 344 | 100 |
| 569 | gi8096476 | Homo sapiens | mRNA for Nop10p, complete cds. | 344 | 100 |
| 569 | gi14424489 | Homo sapiens | , nucleolar protein family A, member 3 (H/ACA small nucleolar RNPs), clone MGC:19486, mRNA, complete cds. | 344 | 100 |
| 570 | gi11595476 | Homo sapiens | mRNA for RPB11b1beta protein (POLR2J2 gene). | 633 | 100 |
| 570 | AAB58870 | Homo sapiens | Breast and ovarian cancer associated antigen protein sequence SEQ ID 578. | 409 | 100 |
| 570 | gi11595474 | Homo sapiens | mRNA for RPB11b1alpha protein (POLR2J2 gene). | 247 | 97 |
| 571 | gi7239381 | Homo sapiens | guanine nucleotide exchange factor smgGDS (RAP1GDS1) mRNA, alternatively spliced, complete cds. | 2995 | 99 |
| 571 | gi13]11713 | Homo sapiens | , RAP1, GTP-GDP dissociation stimulator 1, clone MGC:2897, mRNA, complete cds. | 2994 | 99 |
| 571 | gi6942013 | Homo sapiens | exchange factor smgGDS mRNA, complete cds, alternatively spliced. | 2991 | 99 |
| 572 | gi 12002978 | Homo sapiens | mitosin-associated protein MITAP1 (MITAP1) mRNA, complete cds. | 1736 . | 100 |
| 572 | gi12043569 | Homo sapiens | Nudel mRNA, complete cds. | 1736 | 100 |
| 572 | gi13775593 | Homo sapiens | endooligopeptidase A mRNA, complete cds. | 1720 | 99 |
| 573 | gi7022325 | Homo sapiens | cDNA FLJ10350 fis, clone NT2RM2001131. | 1243 | 100 |
| 573 | gi12052730 | Homo sapiens | mRNA; cDNA DKFZp761F19121 (from clone DKFZp761F19121). | 1243 | 100 |
| 573 | gi3417386 | Mus musculus | microtubule-associated protein, MAP-115 | 428 | 48 |
| 574 | gi7022502 | Homo sapiens | cDNA FLJ10458 fis, clone NT2RP1001457, highly similar to Homo sapiens partial mRNA for beta-transducin family protein. | 2555 | 100 |
| 574 | gi3687833 | Xenopus laevis | notchless | 2149 | 82 |
| 574 | gi12643028 | Oryza sativa | Putative Notchless protein homolog | 1110 | 52 |
| 575 | AAY51115 | Homo sapiens | Human HSEC6 protein. | 3767 | 99 |
| 575 | gi1163174 | Rattus norvegicus | similar to yeast Sec6p, Swiss-Prot Accession Number P32844; similar to mammalian B94, Swiss-Prot Accession Number Q03169; Method: conceptual translation supplied by author | 3606 | 94 |
| 575 | AAB49655 | Homo sapiens | Human SEC7 protein sequence SEQ ID 14. | 2737 | 89 |
| 576 | gi7020303 | Homo sapiens | cDNA FLJ20300 fis, clone HEP06465. | 1697 | 99 |
| 576 | AAB67575 | Homo sapiens | Amino acid sequence of a human hydrolytic enzyme HYENZ7. | 759 | 47 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|-------------------------------|--|-------|---------------|
| 576 | gi10434892 | Homo sapiens | cDNA FLJ13055 fis, clone NTZRP3001538, weakly similar to HYPOTHETICAL 39.0 KD PROTEIN T28D9.3 IN CHROMOSOME II. | 755 | 47 |
| 577 | AAR15222 | Homo sapiens | Chronic myelogenous leukaemia-derived myeloid-related protein. | 513 | 100 |
| 577 | gi32402 | Homo sapiens | Human mRNA for HP-1, a member of the corticostatin/defensin family. | 493 | 100 |
| 577 | gi181527 | Homo sapiens | Human neutrophil peptide (defensin) 1 mRNA, complete cds. | 493 | 100 |
| 578 | AAY41716 | Homo sapiens | Human PRO860 protein sequence. | 5224 | 100 |
| 578 | AAB44272 | Homo sapiens | Human PRO860 (UNQ421) protein sequence SEQ ID NO:211. | 5224 | 100 |
| 578 | gi14042832 | Homo sapiens | cDNA FLJ14946 fis, clone PLACE2000034, weakly similar to LAR PROTEIN PRECURSOR (EC 3.1.3.48). | 3746 | 93 |
| 579 | gi7021880 | Homo sapiens | cDNA FLJ10054 fis, clone HEMBA1001310. | 2306 | 100 |
| 579 | gi12653981 | Homo sapiens | , TRIAD3 protein, clone MGC:998, mRNA, complete cds. | 2306 | 100 |
| 579 | gi7109299 | Homo sapiens | TRIAD3 mRNA, partial cds. | 2013 | 100 |
| 580 | gi3288457 | Homo sapiens | mRNA for C2 domain containing PI3- kinase. | 7615 | 99 |
| 580 | gi3059227 | Rattus norvegicus | phosphoinositide 3-kinase • | 3988 | 80 |
| 580 | gi3041786 | Mus musculus | Phosphoinositide 3-Kinase-C2gamma | 3984 | 78 |
| 581 | gi10437125 | Homo sapiens | cDNA: FLJ21103 fis, clone CAS04883. | 1802 | 99 |
| 581 | gi7020867 | Homo sapiens | cDNA FLJ20635 fis, clone KAT03466. | 786 | 52 |
| 582 | gi13937952 | Homo sapiens | , Similar to upregulated during skeletal muscle growth 5, clone MGC:14697, mRNA, complete cds. | 297 | 100 |
| 582 | gi6851054 | Rattus norvegicus | DAPIT protein | 278 | 91 |
| 582 | gi9843791 | Mus musculus | stretch regulated skeletal muscle protein | 259 | 84 |
| 583 | gi7582286 | Homo sapiens | BM-007 | 599 | 100 |
| 583 | AAG02907 | Homo sapiens | Human secreted protein, SEQ ID NO: 6988. | 477 | 98 |
| 583 | gi3878572 | Caenorhabditis elegans | M01F1.6 | 161 | 28 |
| 584 | gi13477103 | Homo sapiens | , clone MGC:1012, mRNA, complete cds. | 3001 | 99 |
| 584 | gi12052999 | Homo sapiens | mRNA; cDNA DKFZp434E1711 (from clone DKFZp434E1711); complete cds. | 2619 | 98 |
| 584 | gi7020996 | Homo sapiens | cDNA FLJ20721 fis, clone HEP15722. | 2402 | 100 |
| 585 | AAW48892 | Homo sapiens | Human guanylate binding protein B (HGBPB). | 2645 | 94 |
| 585 | gi12803663 | Homo sapiens | , guanylate binding protein 1, interferon- inducible, 67kD, clone MGC:3949, mRNA, complete cds. | 2000 | 66 |
| 585 | gi183002 | Homo sapiens | Human guanylate binding protein isoform I (GBP-2) mRNA, complete cds. | 2000 | 66 |
| 586 | gi7023366 | Homo sapiens | cDNA FLJ10983 fis, clone PLACE1001781, weakly similar to PROBABLE PHOSPHOMANNOMUTASE (EC 5.4.2.8). | 3218 | 99 |
| 586 | gi12052930 | Homo sapiens | mRNA; cDNA DKFZp566B1524 (from clone DKFZp566B1524); complete cds. | 3216 | 99 |
| 586 | gi3395586 | Schizosacchar omyces pombe | similarity to phosphomannomutases | 1211 | 43 |

| SEQ ID | Accession | Species | Description | Score | % |
|------------|-------------------------|------------------------------|---|-------|----------|
| NO: | No. | ļ., | 37.10 | | Identity |
| 587 587 | gi13537208 gi2440074 | Mus musculus Homo sapiens | Mel18 and Bmil like ring finger mRNA for RNF3A (DONG1) ring finger | 347 | 37 |
| | | | protein. | | |
| 587 | gi13537206 | Homo sapiens | hMBLR mRNA, complete cds. | 345 | 40 |
| 588 | gi14042249 | Homo sapiens | cDNA FLJ14610 fis, clone | 2797 | 99 |
| | | | NT2RP1000958, weakly similar to | | |
| 588 | gi14042246 | | AUTOANTIGEN NGP-1. cDNA FLJ14608 fis, clone | 2741 | 99 |
| 300 | g114042246 | Homo sapiens | NT2RP1000915, weakly similar to | 2/41 | 99 |
| | 1 | | AUTOANTIGEN NGP-1. | | { |
| 588 | gi6457340 | Homo sapiens | E2IG3 (E2IG3) mRNA, complete cds. | 2650 | 100 |
| 589 | gi7020925 | Homo sapiens | cDNA FLJ20673 fis, clone KAIA4464. | 2232 | 100 |
| 589 | gi7682684 | Homo sapiens | phosphoprotein associated with GEMs | 2222 | 99 |
| | g | | (PAG) mRNA, complete cds. | | 1 |
| 589 | gi7707799 | Rattus | Csk binding protein Cbp | 1696 | 78 |
| | _ | norvegicus | | | l |
| 590 | gi6682873 | Homo sapiens | rec mRNA, complete cds. | 2002 | 100 |
| 590 | gi7230612 | Rattus | small rec | 1916 | 95 |
| | | norvegicus | | | L |
| 590 | gi3881771 | Caenorhabditis | contains similarity to Pfam domain: | 586 | 39 |
| | | elegans | PF01529 (DHHC zinc finger domain), | | |
| 591 | gi439522 | Mus musculus | Score=137.4, E-value=8.4e-38, N=1 ribosomal protein S3 | 678 | 100 |
| 591 | gi57728 | Rattus rattus | ribosomal protein S3 (AA 1-243) | 678 | 100 |
| 591 | gi13111933 | Homo sapiens | , ribosomal protein S3, clone MGC:3657. | 678 | 100 |
| | 8 | Axome suprems | mRNA, complete cds. | 0.0 | 1.00 |
| 592 | gi6599070 | Homo sapiens | mRNA for LIM domains containing | 3675 | 99 . |
| 592 | -:(600207 | 14 | protein 1. | 2728 | 76 |
| 592 | gi6599307 gi13548632 | Mus musculus Homo sapiens | LIM domains containing protein 1 partial LIMD1 gene for LIM domains | 2690 | 99 |
| 392 | g113348632 | FIGING Sapiens | containing 1, exons 1-2, complete | 2090 | 1 33 |
| | | | sequence. | | |
| 593 | gi7020974 | Homo sapiens | cDNA FLJ20706 fis, clone KAIA1273. | 2824 | 98 |
| 593 | gi12082725 | Mus musculus | B cell phosphoinositide 3-kinase adaptor | 411 | 29 |
| 593 | AAG02945 | Homo sapiens | Human secreted protein, SEQ ID NO: 7026. | 526 | 100 |
| 594 | gi11596144 | Homo sapiens | STE20-like kinase mRNA, partial cds. | 5159 | 99 |
| 594 | gi3452473 | Rattus | serine/threonine protein kinase TAO1 | 5117 | 98 |
| | B | norvegicus | | | 1 |
| 594 | AAY55937 | Homo sapiens | Human SULU3 protein. | 4045 | 100 |
| 595 | gi695802 | Homo sapiens | transcription factor SL1 mRNA, partial | 1693 | 99 |
| | | | cds. | | |
| 595 | gi1842206 | Mus musculus | TAFI68 | 1326 | 76 |
| 596 | gi7020363 | Homo sapiens | cDNA FLJ20335 fis, clone HEP11429. | 2940 | 99 |
| 596 | AAB65680 | Homo sapiens | Novel protein kinase, SEQ ID NO: 208. | 2940 | 99 |
| 596 | AAB32078 | Homo sapiens | Human secreted protein BLAST search protein SEQ ID NO: 136. | 826 | 100 |
| 597 | gi7020747 | Homo sapiens | cDNA FLJ20558 fis, clone KAT11870. | 2990 | 100 |
| 597 | gi12053175 | Homo sapiens | mRNA; cDNA DKFZp434A172 (from | 2990 | 100 |
| | | | clone DKFZp434A172); complete cds. | | |
| 597 | gi10439123 | Homo sapiens | cDNA: FLJ22650 fis, clone HSI07344. | 2166 | 100 |
| 598 | gi7023601 | Homo sapiens | cDNA FLJ11127 fis, clone PLACE1006225. | 1897 | 100 |
| 598 | gi12224968 | Homo sapiens | mRNA; cDNA DKFZp667E105 (from | 620 | 100 |
| - | | | clone DKFZp667E105). | | 1 |
| | gi14043433 | Homo sapiens | , clone IMAGE:3952677, mRNA, partial | 549 | 41 |
| 598 | - | | | | |
| 598 | gi6483296 | Homo sapiens | CDH9 mRNA for cadherin-9, complete | 4132 | 100 |

| SEQ ID | Accession | Species | Description | Score | % |
|--------|------------|------------------------|--|----------|----------|
| NO: | No. | | | <u> </u> | Identity |
| 599 | gi867999 | Gallus gallus | chicken cadherin-6B | 3044 | 72 |
| 599 | gi974185 | Homo sapiens | mRNA for cadherin-6, complete cds. | 3032 | 72 |
| 600 | gi5734605 | Homo sapiens | mRNA for KARP-1-binding protein 3, complete cds. | 750 | 51 |
| 600 | gi5734601 | Homo sapiens | mRNA for KARP-1-binding protein 1 (KAB1), complete cds. | 750 | 51 |
| 600 | gi5734603 | Homo sapiens | mRNA for KARP-1-binding protein 2 (KAB2), complete cds. | 750 | 51 |
| 601 | gi10434848 | Homo sapiens | cDNA FLJ13028 fis, clone NT2RP3001055, weakly similar to Drosophila melanogaster separation anxiety protein (san) mRNA. | 889 | 100 |
| 601 | gi10435107 | Homo sapiens | cDNA FLJ13194 fis, clone NT2RP3004378, weakly similar to Drosophila melanogaster separation anxiety protein (san) mRNA. | 889 | 100 |
| 601 | AAB56739 | Homo sapiens | Human prostate cancer antigen protein sequence SEQ ID NO:1317. | 874 | 98 |
| 602 | gi13325182 | Homo sapiens | , clone IMAGE:3638994, mRNA, partial cds. | 897 | 100 |
| 602 | gi12654203 | Homo sapiens | , clone IMAGE:3449323, mRNA, partial cds. | 560 | 100 |
| 602 | gi4514314 | Bacillus halodurans | YlqF | 260 | 39 |
| 603 | gi10954046 | Homo sapiens | oxidation protection protein (OXR1) mRNA, complete cds. | 1034 | 97 |
| 603 | gi13540300 | Mus musculus | nucleolar protein C7B | 1431 | 94 |
| 603 | gi7021988 | Homo sapiens | cDNA FLJ10125 fis, clone HEMBA1002954. | 1441 | 99 |
| 604 | gi1150495 | Mus musculus | homology to nucleosome assembly proteins; specifically expressed in neurons | 211 | 36 |
| 604 | gi1161252 | Glycine max | nucleosome assembly protein 1 | 136 | 40 |
| 604 | gi5931610 | Homo sapiens | mRNA for Nucleosome Assembly Protein 1-like 2, complete cds. | 196 | 37 |
| 605 | gi7547029 | Homo sapiens | GAP-like protein (N61) mRNA, complete cds. | 4684 | 99 |
| 605 | gi7688683 | Homo sapiens | kinesin heavy chain-like protein (KHCHP) mRNA, complete cds. | 822 | 100 |
| 605 | AAG03378 | Homo sapiens | Human secreted protein, SEQ ID NO: 7459. | 633 | 99 |
| 606 | gi7022593 | Homo sapiens | cDNA FLJ10511 fis, clone NT2RP2000656. | 1425 | 100 |
| 606 | gi12224996 | Homo sapiens | mRNA; cDNA DKFZp667G248 (from clone DKFZp667G248). | 1031 | 100 |
| 606 | gi10436327 | Homo sapiens | cDNA FLJ13991 fis, clone Y79AA1002115. | 803 | 100 |
| 607 | gi8885998 | Rattus norvegicus | neuronal C-SRC tyrosine-specific protein kinase | 2826 | 98 |
| 607 | gi201057 | Mus musculus | tyrosine-specific protein kinase | 2822 | 98 |
| 607 | gi338460 | Homo sapiens | Human c-src-1 proto-oncogene, exon 12. | 2815 | 98 |
| 608 | gi7243633 | Homo sapiens | RB-associated KRAB repressor (RBAK) mRNA, complete cds. | 3993 | 100 |
| 608 | gi7243635 | Mus musculus | RB-associated KRAB repressor | 3025 | 78 . |
| 608 | gi10434235 | Homo sapiens | cDNA FLJ12629 fis, clone NT2RM4001828, moderately similar to | 1881 | 73 |
| 400 | | L | ZINC FINGER PROTEIN 84. | 000 | |
| 609 | gi7008402 | Homo sapiens | kappa B-ras i mRNA, complete cds. | 982 | 100 |
| 609 | gi14042659 | Homo sapiens | cDNA FLJ14843 fis, clone | 978 | 99 |

WO 02/22660 PCT/US01/26015

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|----------------------------|--|-------|---------------|
| | | | PLACE1000040, weakly similar to TRANSFORMING PROTEIN P21/K- RAS 2B. | | |
| 609 | gi7239257 | Mus musculus | kappaB-Ras1 | 952 | 94 |
| 610 | gi13625164 | Homo sapiens | ankyrin mRNA, complete cds. | 426 | 100 |
| 610 | gi12698638 | Homo sapiens | ankyrin-repeat family A protein 2 (ANKRA2) mRNA, complete cds. | 426 | 100 |
| 610 | gi10434525 | Homo sapiens | cDNA FLJ12814 fis, clone NT2RP2002520, weakly similar to Homo sapiens transcription factor RFX-B (RFXB) mRNA. | 426 | 100 |
| 611 . | gi7959841 | Homo sapiens | PRO1853 | 510 | 100 |
| 611 | AAG01282 | Homo sapiens | Human secreted protein, SEQ ID NO: 5363. | 301 | 100 |
| 612 | gi5757703 | Mus musculus | syntrophin-associated serine-threonine protein kinase | 7464 | 92 |
| 612 | gi13537204 | Homo sapiens | mRNA for MAST205, complete cds. | 4616 | 68 |
| 612 | gi406058 | Mus musculus | protein kinase | 4569 | 65 |
| 613 | gi7020724 | Homo sapiens | cDNA FLJ20545 fis, clone KAT11476. | 1780 | 100 |
| 613 | AAB63186 | Homo sapiens | Human secreted protein sequence encoded by gene 3 SEQ ID NO:112. | 1693 | 100 |
| 613 | gi7243701 | Drosophila melanogaster | WDS | 1574 | 91 |
| 614 | gi13383476 | Homo sapiens | NUB1 (NUB1) mRNA, complete cds. | 3109 | 100 |
| 614 | gi5360093 | Homo sapiens | NY-REN-18 antigen mRNA, complete cds. | 2958 | 95 |
| 614 | gi863014 | Mus musculus | BS4 peptide | 2671 | 84 |
| 615 | AAB87345 | Homo sapiens | Human gene 4 encoded secreted protein HDPFY41, SEQ ID NO:86. | 4534 | 100 |
| 615 | gi4886489 | Homo sapiens | mRNA; cDNA DKFZp564L2123 (from clone DKFZp564L2123); partial cds. | 2892 | 99 |
| 615 | gi12711793 | Homo sapiens | estrogen regulated LIV-1 protein (LIV-1) mRNA, complete cds. | 1171 | 39 |
| 616 | gi7638247 | Homo sapiens | mesenchymal stem cell protein DSCD75 mRNA, complete cds. | 1063 | 100 |
| 616 | gi12654929 | Homo sapiens | , mesenchymal stem cell protein DSCD75, clone MGC:5515, mRNA, complete cds. | 1063 | 100 |
| 616 | AAB03956 | Homo sapiens | Human mesenchymal stem cell polypeptide. | 1063 | 100 |
| 617 | gi7582304 | Homo sapiens | BM-016 | 584 | 100 |
| 617 | AAW78199 | Homo sapiens | Human secreted protein encoded by gene 74 clone HGBAC11. | 562 | 98 |
| 617 | AAW85610 | Homo sapiens | Secreted protein clone eh80_1. | 562 | 98 |
| 618 | gi13603398 | Homo sapiens | mRNA for SEZ6L, complete cds. | 4199 | 98 |
| 618 | gi13185723 | Homo sapiens | n 1755 can be A, G, C, or T | 2164 | 49 |
| 618 | AAB70537 | Homo sapiens | Human PRO7 protein sequence SEQ ID NO:14. | 2164 | 49 |
| 619 | gi3880445 | Caenorhabditis elegans | contains similarity to Pfam domain: PF02214 (K+ channel tetramerisation domain), Score=79.5, E-value=2.3e-20, N=1 | 327 | 40 |
| 619 | AAY34129 | Homo sapiens | Human potassium channel K+Hnov28. | 195 | 40 |
| 619 | AAZ11907_ aal | Homo sapiens | Human potassium channel K+Hnov28 cDNA (5' splice variant 1). | 195 | |
| 620 | gi10437116 | Homo sapiens | cDNA: FLJ21097 fis, clone CAS03931. | 1146 | 100 |
| 620 | gi14250732 | Homo sapiens | , chromosome 11 open reading frame 14, clone MGC:12847, mRNA, complete cds. | 1146 | 100 |
| 620 | gi13276621 | Homo sapiens | mRNA; cDNA DKFZp761G1913 (from | 378 | 43 |

| SEQ ID | Accession | Species | Description | Score | % |
|--------|-------------|-------------------------------|--|--------|----------|
| NO: | No. | Species | Description | | Identity |
| | | | clone DKFZp761G1913). | | |
| 621 | gi10437078 | Homo sapiens | cDNA: FLJ21069 fis, clone CAS01594. | 955 | 58 |
| 621 | gi5911935 | Homo sapiens | mRNA; cDNA DKFZp586N1922 (from clone DKFZp586N1922); partial cds. | 867 | 100 |
| 621 | AAB27870 | Homo sapiens | Protein fragment encoded by gene 27. | 657 | 100 |
| 622 | gi13097159 | Homo sapiens | , tumor protein, translationally-controlled 1, clone MGC:5308, mRNA, complete cds. | 898 | 100 |
| 622 | gi14043771 | Homo sapiens | , clone MGC:14243, mRNA, complete cds. | 898 | 100 |
| 622 . | gi7573519 | Homo sapiens | TPT1 gene for translationally controlled tumor protein (TCTP), exons 1-6. | 898 | 100 |
| 623 | gi7020339 · | Homo sapiens | cDNA FLJ20320 fis, clone HEP08923. | 1135 | 100 |
| 623 | AAB18972 | Homo sapiens | Amino acid sequence of a human transmembrane protein. | 1135 | 100 |
| 623 | gi1314162 | Schizosacchar omyces pombe | seven transmembrane protein | 217 | 29 |
| 624 | gi6467990 | Mus musculus | PDZ domain actin binding protein Shroom | 4816 | 66 |
| 624 | gi6467992 | Mus musculus | actin binding protein ShroomS | 4816 | 66 |
| 624 | gi13938323 | Homo sapiens | , Similar to shroom, clone IMAGE:3349317, mRNA, partial cds. | 4006 | 99 |
| 625 | gi12804029 | Homo sapiens | , clone IMAGE:3940519, mRNA, partial cds. | 1551 | 100 |
| 625 | AAY21850 | Homo sapiens | Human signal peptide-contianing protein (SIGP) (clone ID 1880830). | 1109 . | 100 |
| 625 | gi8655657 | Homo sapiens | mRNA; cDNA DKFZp762O076 (from clone DKFZp762O076). | 593 | 57 |
| 626 | gi7328140 | Homo sapiens | mRNA; cDNA DKFZp762D096 (from clone DKFZp762D096); partial cds. | 601 | 100 |
| 626 | gi13436341 | Homo sapiens | , Similar to RIKEN cDNA 1600014C10 gene, clone MGC:10922, mRNA, complete cds. | 384 | 100 |
| 627 | gi1293559 | Mus musculus | astrotactin | 4312 | 95 |
| 627 | gi6502571 | Mus musculus | astrotactin2 | 2580 | 51 |
| 627 | gi6502573 | Homo sapiens | astrotactin2 (ASTN2) mRNA, complete cds. | 2569 | 51 |
| 628 | AAY73387 | Homo sapiens | HTRM clone 3340290 protein sequence. | 1439 | 95 |
| 628 | AAY48312 | Homo sapiens | Human prostate cancer-associated protein 9. | 1073 | 84 |
| 628 | gi12654077 | Homo sapiens | , clone IMAGE:3458173, mRNA, partial cds. | 1045 | 86 |
| 629 | gi11095188 | Homo sapiens | dipeptidyl peptidase 8 (DPP8) mRNA, complete cds. | 3521 | 99 |
| 629 | gi14042790 | Homo sapiens | cDNA FLJ14920 fis, clone PLACE1007416, weakly similar to DIPEPTIDYL PEPTIDASE IV (EC 3.4.14.5). | 2457 | 99 |
| 629 | gi7020273 | Homo sapiens | cDNA FLJ20283 fis, clone HEP04088. | 2483 | 100 |
| 630 | gi11095188 | Homo sapiens | dipeptidyl peptidase 8 (DPP8) mRNA, complete cds. | 2560 | 99 |
| 630 | gi14042790 | Homo sapiens | cDNA FLJ14920 fis, clone PLACE1007416, weakly similar to DIPEPTIDYL PEPTIDASE IV (EC 3.4.14.5). | 2457 | 99 |
| 630 | gi11095192 | Homo sapiens | dipeptidyl peptidase 8 (DPP8) mRNA, partial cds, alternatively spliced. | 2482 | 100 |
| 631 | gi7020611 | Homo sapiens | cDNA FLJ20481 fis, clone KAT07534. | 2211 | 99 |
| 631 | AAY57908 | Homo sapiens | Human transmembrane protein HTMPN- | 975 | 44 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|-----------------------------|--|--------|---------------|
| 110. | 1.0. | | 32. | | |
| 631 | AAB54284 | Homo sapiens | Human pancreatic cancer antigen protein sequence SEQ ID NO:736. | 516 | 40 |
| 632 | gi35700 | Homo sapiens | Human mRNA for phosphoriobosyl pyrophosphate synthetase subunit II (EC 2.7.6.1). | 1596 | 99 |
| 632 | gi206434 | Rattus norvegicus | phosphoribosyl pyrophosphate synthetase II | 1585 | 98 |
| 632 | gi56979 | Rattus norvegicus | ribose-phosphate pyrophosphokinase subunit II (AA 1-318) | 1585 | 98 |
| 633 | gi11181620 | Homo sapiens | Rag D mRNA, complete cds. | 1276 | 100 |
| 633 | gi6808148 | Homo sapiens | mRNA; cDNA DKFZp761H171 (from clone DKFZp761H171); partial cds. | 1276 | 100 |
| 633 | AAB56443 | Homo sapiens | Human prostate cancer antigen protein sequence SEQ ID NO:1021. | 1276 | 100 |
| 634 | gi6807893 | Homo sapiens | mRNA; cDNA DKFZp434H2226 (from clone DKFZp434H2226); partial cds. | 1079 | 100 |
| 635 | gi 10435042 | Homo sapiens | cDNA FLJ13152 fis, clone NT2RP3003385, highly similar to Mus musculus SKD3 mRNA. | 3495 | 100 |
| 635 | gi4958935 | Rattus norvegicus | suppressor of potassium transport defect 3 | 3085 | 88 |
| 635 | gi563129 | Mus musculus | SKD3 | 3066 | 88 |
| 636 | AAB20322 | Homo sapiens | Human protein phosphatase and kinase protein-1. | 1770 | 100 |
| 636 | gi1903458 | Dictyostelium discoideum | myosin heavy chain kinase B | 236 | 32 |
| 636 | gi2104701 | Mus musculus | elongation factor-2 kinase | 199 | 29 |
| 637 | gi7670003 | Homo sapiens | mRNA; cDNA DKFZp434P0531 (from clone DKFZp434P0531). | 1850 | 100 |
| 637 | gi7417474 | Homo sapiens | chromosome 14 clone RP11-493G17 and CTD-2516D11 map 14q24.3, complete sequence. | 1251 . | 49 |
| 637 | gi7018538 | Homo sapiens | mRNA; cDNA DKFZp434P0111 (from clone DKFZp434P0111); partial cds. | 330 | 43 |
| 638 | gi7022367 | Homo sapiens | cDNA FLJ10375 fis, clone NT2RM2001950. | 3056 | 100 |
| 638 | AAY53026 | Homo sapiens | Human secreted protein clone cn922_5 protein sequence SEQ ID NO:58. | 1752 | 95 |
| 638 | gi4336692 | Drosophila melanogaster | Abnormal X segregation | 816 | 37 |
| 639 | gi7020972 | Homo sapiens | cDNA FLJ20705 fis, clone KA1A1571. | 3641 | 99 |
| 639 | gi12007334 | Homo sapiens | IRS-1 PH domain binding protein PHIP mRNA, complete cds. | 3632 | 99 |
| 639 | gi14286226 | Homo sapiens | , pleckstrin homology domain interacting protein, clone MGC:15187, mRNA, complete cds. | 3632 | 99 |
| 640 | gi7689025 | Homo sapiens | uncharacterized hypothalamus protein HT013 mRNA, complete cds. | 978 | 96 |
| 641 | gi9937505 | Homo sapiens | PLIC-2 mRNA, complete eds. | 3167 | 100 |
| 641 | gi6563288 | Homo sapiens | ubiquitin-like product Chap1/Dsk2 mRNA, complete cds. | 3162 | 99 |
| 641 | AAB47122 | Homo sapiens | Human Chap1. | 3162 | 99 |
| 642 | AAY53001 | Homo sapiens | Human secreted protein clone dn834_1 protein sequence SEQ ID NO:8. | 811 | 100 |
| 642 | AAG01114 | Homo sapiens | Human secreted protein, SEQ ID NO: 5195. | 641 | 99 |
| 642 | gi12652989 | Homo sapiens | , clone MGC:2495, mRNA, complete cds. | 489 | 57 |
| 643 | gi7021064 | Homo sapiens | cDNA FLJ20761 fis, clone HEP00317. | 2240 | 100 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|------------------------------|---|-------|---------------|
| 643 | gi10438264 | Homo sapiens | cDNA: FLJ22019 fis, clone HEP07982. | 2187 | 98 |
| 643 | gi577428 | Rattus norvegicus | Ca2+-dependent activator protein; calcium-dependent actin-binding protein | 1787 | 77 |
| 644 | gi7023651 | Homo sapiens | cDNA FLJ11159 fis, clone PLACE1006966. | 2865 | 99 |
| 644 | gi7023118 | Homo sapiens | cDNA FLJ10835 fis, clone NT2RP4001210. | 1253 | 100 |
| 644 | gi600058 | Saccharomyce s cerevisiae | N1342 | 710 | 39 |
| 645 | gi7020012 | Homo sapiens | cDNA FLJ20121 fis, clone COL05942. | 1334 | 99 |
| 646 | gi14336697 | Homo sapiens | 16p13.3 sequence section 2 of 8. | 609 | 100 |
| 646 | gi13436122 | Homo sapiens | , non-metastatic cells 4, protein expressed in, clone MGC:11088, mRNA, complete cds. | 609 | 100 |
| 646 | gi1945762 | Homo sapiens | H.sapiens mRNA for nucleoside- diphosphate kinase. | 609 | 100 |
| 647 | AAB24225 | Homo sapiens | Human vesicle associated protein 4 SEQ ID NO:4. | 2946 | 99 |
| 647 | gi10439139 | Homo sapiens | cDNA: FLJ22662 fis, clone HSI08080. | 2703 | 99 |
| 647 | AAB58427 | Homo sapiens | Lung cancer associated polypeptide sequence SEQ ID 765. | 1711 | 99 |
| 648 | gi7020604 | Homo sapiens | cDNA FLJ20477 fis, clone KAT07271. | 2639 | 99 |
| 648 | gi6672090 | Drosophila melanogaster | Vegetable | 578 | 32 |
| 649 | gi12802986 | Homo sapiens | , ring finger protein 24, clone MGC:1815, mRNA, complete cds. | 811 | 100 |
| 649 | gi5420200 | Homo sapiens | Novel human mRNA from chromosome 20, similar to SW:GOL1_DROME Q06003 GOLIATH PROTEIN. | 811 | 100 |
| 649 | gi5102892 | Homo sapiens | mRNA full length insert cDNA clone EUROIMAGE 566628. | 566 | 100 |
| 650 | gi6841346 | Homo sapiens | HSPC054 | 497 | 98 |
| 651 | gi7209305 | Homo sapiens | mRNA for FLJ00002 protein, partial cds. | 7637 | 100 |
| 651 | gi6599226 | Homo sapiens | mRNA; cDNA DKFZp434L0827 (from clone DKFZp434L0827); partial cds. | 3519 | 100 |
| 651 | gi10440406 | Homo sapiens | mRNA for FLJ00036 protein, partial cds. | 3457 | 99 |
| 652 | gi7018505 | Homo sapiens | mRNA; cDNA DKFZp434E2220 (from clone DKFZp434E2220). | 2470 | 100 |
| 652 | gi14042579 | Homo sapiens | cDNA FLJ14796 fis, clone NT2RP4001235. | 2466 | 99 |
| 652 | gi7018507 | Homo sapiens | mRNA; cDNA DKFZp434O0420 (from clone DKFZp434O0420). | 2466 | 99 |
| 653 | gi552196 | Plasmodium lophurae | histidine-rich protein | 192 | 40 |
| 653 | gi160362 | Plasmodium falciparum | knob protein | 178 | 42 |
| 653 | gi3845095 | Plasmodium falciparum | knob-associated His-rich protein | 172 | 40 |
| 654 | AAY70539 | Homo sapiens | Human Factor 8 Homologue. | 1353 | 83 |
| 654 | gi14043498 | Homo sapiens | , Similar to neuropilin 1, clone MGC:12920, mRNA, complete cds. | 189 | 34 |
| 654 | gi7271465 | Homo sapiens | soluble neuropilin-1 mRNA, complete cds. | 189 | 34 |
| 655 | gi7019959 | Homo sapiens | cDNA FLJ20087 fis, clone COL03793. | 3964 | 100 |
| 655 | gi13569705 | Homo sapiens | channel kinase 2 (CHAK2) mRNA, complete cds. | 3942 | 99 |
| 655 | AAY95433 | Homo sapiens | Human calcium channel SOC-2/CRAC-1 C-terminal polypeptide. | 1172 | 71 |
| 656 | gi6094668 | Homo sapiens | BAC clone RP11-343N14 from 2, | 208 | 100 |

| gi10435833 | | complete sequence. | | |
|-------------|--|--|------------|------------|
| gi10435833 | | | | |
| | Homo sapiens | cDNA FLJ13729 fis, clone | 208 | 100 |
| | - | PLACE3000121, weakly similar to | | |
| | | VESICULAR TRAFFIC CONTROL | l | 1 |
| | | PROTEIN SEC15. | | |
| gi2827162 | | rsec15 | 160 | 73 |
| | | | | |
| gi10434153 | Homo sapiens | | 1806 | 99 |
| | | N12RM4001116, weakly similar to | l | l . |
| | | | | |
| | <u> </u> | | | |
| gi12053255 | Homo sapiens | | 1806 | 99 |
| 14001000 | | | | |
| gi590 j 808 | | BcDNA.GH03694 | 619 | 56 |
| | | D. C. DVIA | 0000 | 100 |
| | | | | 100 |
| gi12007486 | Homo sapiens | | 2069 | 99 |
| | | | 2020 | 98 |
| | | | | |
| | | | | 40 |
| gi2440074 | Homo sapiens | | 347 | 37 |
| :10 500000 | ** | | 245 | 40 |
| | | | | |
| g1/023690 | Homo sapiens | | 1043 | 99 |
| 10000000 | · · · · · · · · · · · · · · · · · · · | | 0.550 | 100 |
| | | | | 99 |
| gil 1992034 | | antisense KNA overlapping MCH protein | 1609 | 65 |
| AADCCCAC | | 71 | 015 | 98 |
| AAB30040 | Homo sapiens | | 913 | 1 20 |
| ai12052257 | Uomo coniene | | 900 | 100 |
| g112033337 | rionio sapiens | | 1 200 | 100 |
| A A D 26508 | Homo raniene | | 701 | 59 |
| AADJOJJO | Tromo sapiens | | 1,71 | " |
| A A W93947 | Homo saniens | | 1732 | 100 |
| | | | 1 | 1 |
| gi3288459 | Homo sapiens | | 1673 | 100 |
| S | | TFIIS.h. | | |
| gi3288547 | Mus musculus | transcription elongation factor TFIIS.h | 1543 | 90 |
| gi14042893 | Homo sapiens | cDNA FLJ14984 fis, clone | 3478 | 100 |
| _ | | Y79AA1000349, highly similar to | 1 | ł |
| | l . | M.musculus Spnr mRNA for RNA | i . | l |
| | | | | |
| gi13377630 | Homo sapiens | | 3459 | 99 |
| | | | | |
| gi12053237 | Homo sapiens | | 3406 | 100 |
| | | | | |
| gi10436573 | Homo sapiens | | 4423 | 99 |
| | | | 1 | |
| | | | l | ł |
| · | | | | |
| gi10434345 | Homo sapiens | | 4369 | 99 |
| | | | | L |
| | | | | 100 |
| gi9858154 | Homo sapiens | tubby super-family protein (TUSP) | 3598 | 100 |
| | I | mRNA, complete cds, alternatively | 1 | 1 |
| | 1 | | | |
| gi9502082 | Homo sapiens | spliced. tubby super-family protein (TUSP) | 3556 | 100 |
| | gi14042893 gi13377630 gi12053237 gi10436573 gi10434345 AAB27235 | | gi10434153 | gi10434153 |

| SEQ ID | Accession | Species | Description | Score | % Identity |
|--------|------------------|--|---|-------|---------------|
| NO: | No. gi9502080 | Mus musculus | tubby super-family protein | 3505 | 98 |
| 667 | gi7106796 | Homo sapiens | HSPC203 | 554 | 100 |
| 667 | gi9963859 | Homo sapiens | PTD019 mRNA, complete cds. | 554 | 100 |
| 667 | AAY35987 | Homo sapiens | Extended human secreted protein sequence, SEQ ID NO. 236. | 554 | 100 |
| 668 | gi6996442 | Homo sapiens | CTL1 gene. | 3398 | 99 |
| 668 | gi6996589 | Rattus norvegicus | CTL1 protein | 3291 | 96 |
| 668 | gi6996587 | Torpedo marmorata | CTL1 protein | 2454 | 71 |
| 669 | gi6808165 | Homo sapiens | mRNA; cDNA DKFZp761A052 (from clone DKFZp761A052). | 2265 | 100 |
| 669 | gi10439058 | Homo sapiens | cDNA: FLJ22607 fis, clone HSI04846. | 1992 | 100 |
| 669 | gi7673616 | Mus musculus | DXImx46e protein | 1958 | 98 |
| 670 | gi6808252 | Homo sapiens | mRNA; cDNA DKFZp434D1319 (from clone DKFZp434D1319); partial cds. | 2336 | 100 |
| 670 | gi170035 | Glycine max | N-75 | 221 | 27 |
| 670 | gi18576 | Glycine max | pre-pro polypeptide (AA -25 to 284) | 219 | 27 |
| 671 | AAW93947 | Homo sapiens | Human regulatory molecule HRM-3 protein. | 1116 | 99 |
| 671 | gi3288459 | Homo sapiens | mRNA for transcription elongation factor TFIIS.h. | 1057 | 99 |
| 671 | gi3288547 | Mus musculus | transcription elongation factor TFIIS.h | 950 | 86 |
| 672 | gi10434615 | Homo sapiens | cDNA FLJ12875 fis, clone NT2RP2003777. | 1818 | 99 |
| 672 | gi8778741 | Arabidopsis thaliana | T30E16.12 | 254 | 27 |
| 672 | gi6520214 | Arabidopsis thaliana | ZCF61 | 228 | 29 |
| 673 | AAB88424 | Homo sapiens | Human membrane or secretory protein clone PSEC0197. | 3032 | 99 |
| 673 | gi9294464 | Arabidopsis thaliana | long-chain-fatty-acid-CoA ligase-like protein | 581 | 37 |
| 673 | gi699196 | Mycobacteriu m leprae | 4-coumarate-coA ligase | 326 | 45 |
| 674 | gi7022969 | Homo sapiens | cDNA FLJ10747 fis, clone NT2RP3001799. | 3378 | 99 |
| 674 | AAY86211 | Homo sapiens | Nuclear transport protein clone hfb066 protein sequence. | 1432 | 87 |
| 674 | gi10439560 | Homo sapiens | cDNA: FLJ23007 fis, clone LNG00451. | 703 | 100 |
| 675 | gi7021968 | Homo sapiens | cDNA FLJ10111 fis, clone HEMBA 1002696. | 2753 | 99 |
| 675 | gi14017768 | Mus musculus | FLJ10111 | 2214 | 92 |
| 675 | gi10440211 | Homo sapiens | cDNA: FLJ23501 fis, clone LNG02837. | 2160 | 90 |
| 676 | gi7021968 | Homo sapiens | cDNA FLJ10111 fis, clone HEMBA1002696. | 2728 | 98 |
| 676 | gi14017768 | Mus musculus | FLJ10111 | 2200 | 90 |
| 676 | gi10440211 | Homo sapiens | cDNA: FLJ23501 fis, clone LNG02837. | 2237 | 92 |
| 677 | gi7019869 | Homo sapiens | cDNA FLJ20036 fis, clone COL00219. | 2834 | 100 |
| 677 | gi12723779 | Lactococcus lactis subsp. lactis | UNKNOWN PROTEIN | 306 | 35 |
| 677 . | gi8885520 | Streptococcus | streptococcal hemagglutinin | 297 | 29 |
| 678 | gi10437508 | Homo sapiens | cDNA: FLJ21415 fis, clone COL04030. | 1129 | 001 |
| 679 | gi3135314 | Homo sapiens | chromosome 7q22 sequence, complete sequence. | 1226 | 100 |
| 679 | gi6752287 | Homo sapiens | Novel human gene mapping to chomosome X. | 390 | 43 |

| SEQ ID | Accession | Species | Description | Score | % |
|------------|-----------------|--------------------------------|---|-------|-----------------|
| NO: 679 | No. AAB28327 | Homo sapiens | Human secreted protein BLAST search protein SEQ ID NO: 111. | 265 | Identity 100 |
| 680 | gi3135314 | Homo sapiens | chromosome 7q22 sequence, complete sequence. | 1199 | 95 |
| 680 | gi6752287 | Homo sapiens | Novel human gene mapping to chomosome X. | 363 | 41 |
| 680 | AAB28327 | Homo sapiens | Human secreted protein BLAST search protein SEQ ID NO: 111. | 265 | 100 |
| 681 | gi10439089 | Homo sapiens | cDNA: FLJ22626 fis, clone HSI06109. | 2120 | 99 |
| 681 | gi11044557 | Homo sapiens | Human DNA sequence from clone RP11- 42415 on chromosome 6 Contains a novel gene, STSs, GSSs and a CpG island, complete sequence. | 1185 | 64 |
| 681 | gi12654241 | Homo sapiens | , Similar to splicing factor, arginine/serine-rich 4 (SRp75), clone MGC:5283, mRNA, complete cds. | 949 | 98 |
| 682 | gi14042277 | Homo sapiens | cDNA FLJ14626 fis, clone NT2RP2000288. | 3029 | 99 |
| 682 | gi7022410 | Homo sapiens | cDNA FLJ10402 fis, clone NT2RM4000457. | 2279 | 100 |
| 682 | gi6841196 | Homo sapiens | HSPC273 | 1086 | 100 |
| 683 | gi2815604 | Homo sapiens | Opa-interacting protein OIP2 mRNA, partial cds. | 1364 | 100 |
| 683 | AAB63276 | Homo sapiens | Human breast cancer associated antigen protein sequence SEQ ID NO:638. | 839 | 96 |
| 683 | AAB63406 | Homo sapiens | Human breast cancer associated antigen protein sequence SEQ ID NO:768. | 839 | 96 |
| 684 | AAB07228 | Homo sapiens | Human prostate cancer predisposing protein HPC2. | 4325 | 100 |
| 684 | AAY99850 | Homo sapiens | Human sulphatase G. | 4315 | 99 |
| 684 | gi10946497 | Pan troglodytes | ELAC2 | 4283 | 98 |
| 685 | gi7688979 | Homo sapiens | uncharacterized bone marrow protein BM042 | 895 | 100 |
| 685 . | AAB36580 | Homo sapiens | Human FLEXHT-2 protein sequence SEQ ID NO:2. | 895 | 100 |
| 685 | AAB34771 | Homo sapiens | Human secreted protein fragment encoded by DNA clone vq23 1. | 888 | 99 |
| 686 | gi10438990 | Homo sapiens | cDNA: FLJ22559 fis, clone HSI01591. | 1897 | 100 |
| 686 | gi8954034 | Arabidopsis thaliana | F10K1.17 | 162 | 31 |
| 687 | gi7020674 | Homo sapiens | cDNA FLJ20515 fis, clone KAT09889. | 2027 | 100 |
| 687 | AAB20331 | Homo sapiens | Human protein phosphatase and kinase protein-10. | 1472 | 92 |
| 687 | AAB73226 | Homo sapiens | Human phosphatase NP_060746_h. | 576 | 83 |
| 688 | gi6688145 | Homo sapiens | mRNA for NICE-3 protein, clone 1023j12. | 1019 | 100 |
| 688 | gi4689120 | Homo sapiens | HSPC012 | 717 | 93 |
| 688 | gi12655055 | Homo sapiens | , DKFZP586G1722 protein, clone MGC:1147, mRNA, complete cds. | 717 | 93 |
| 689 | gi7023701 | Homo sapiens | cDNA FLJ11190 fis, clone PLACE1007583. | 1317 | 100 |
| 690 | gi6469703 | Mycobacteriu m tuberculosis | DipZ | 203 | 31 |
| 691 | gi13676779 | Mus musculus | Arkadia | 1939 | 93 |
| 691 | gi13752369 | Gallus gallus | ring finger protein | 1888 | 91 |
| 691 | gi13752371 | Xenopus laevis | ring finger-H2 protein | 1537 | 76 |
| 692 | gi458255 | Homo sapiens | Human X-linked PEST-containing | 2849 | 99 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|------------------------------|--|-------|---------------|
| | | | transporter (XPCT) gene, exon 6. | | |
| 692 | gi458247 | Homo sapiens | Human X-linked PEST-containing transporter (XPCT) mRNA, partial cds. | 2766 | 99 |
| 692 | gi2944356 | Mus musculus | X-linked PEST-containing transporter | 2249 | 88 |
| 693 | gi14042736 | Homo sapiens | cDNA FLJ14888 fis, clone PLACE1003762. | 2034 | 99 |
| 693 | gi6841178 | Homo sapiens | HSPC264 | 2019 | 99 |
| 694 | gi7023413 | Homo sapiens | cDNA FLJ11012 fis, clone PLACE1003190, weakly similar to SOF1 PROTEIN. | 2377 | 99 |
| 694 | gi14042745 | Homo sapiens | cDNA FLJ14893 fis, clone PLACE1004302, weakly similar to SOF1 PROTEIN. | 2377 | 99 |
| 694 | gi5912184 | Homo sapiens | mRNA; cDNA DKFZp564O0463 (from clone DKFZp564O0463); partial cds. | 1159 | 99 |
| 695 | gi7022931 | Homo sapiens | cDNA FLJ10724 fis, clone NT2RP3001176. | 2683 | 99 |
| 695 | gi14198202 | Mus musculus | Similar to melanoma antigen recognized by T cells 2 | 2126 | 82 |
| 695 | gi4826524 | Homo sapiens | Novel human gene mapping to chomosome 1. | 982 | 92 |
| 696 | gi7022990 | Homo sapiens | cDNA FLJ10761 fis, clone NT2RP3004669, weakly similar to ETHANOLAMINE KINASE (EC 2.7.1.82). | 2119 | 99. |
| 696 | gi9998952 | Homo sapiens | ethanolamine kinase (EKII) mRNA, complete cds. | 930 | 56 |
| 696 | gi532128 | Drosophila melanogaster | ethanolamine kinase | 525 | 45 |
| 697 | gi186774 | Homo sapiens | Human Kruppel related zinc finger protein (HTF10) mRNA, complete cds. | 986 | 38 |
| 697 | gi5441615 | Canis familiaris | zinc finger protein | 988 | 37 |
| 697 | gi38032 | Homo sapiens | Human ZNF43 mRNA. | 947 | 36 |
| 698 | gi13537202 | Homo sapiens | PC-LKC mRNA for protocadherin LKC, complete cds. | 2877 | 100 |
| 698 . | gi7020017 | Homo sapiens | cDNA FLJ20124 fis, clone COL06056. | 2862 | 99 |
| 698 | AAY01410 | Homo sapiens | Secreted protein encoded by gene 28 clone HE9ND43. | 963 | 100 |
| 699 | gi7688977 | Homo sapiens | uncharacterized bone marrow protein BM041 | 888 | 100 |
| 699 | AAY86515 | Homo sapiens | Human gene 71-encoded protein fragment, SEQ ID NO:430. | 888 | 100 |
| 699 | gi7018421 | Homo sapiens | mRNA; cDNA DKFZp564J157 (from clone DKFZp564J157). | 880 | 99 |
| 700 | gi7209307 | Homo sapiens | mRNA for FLJ00003 protein, partial cds. | 1102 | 93 |
| 700 | gi14276857 | Homo sapiens | PC2-glutamine-rich-associated protein (PCQAP) mRNA, complete cds. | 429 | J |
| 700 | gi14043091 | Homo sapiens | , clone IMAGE:3350171, mRNA, partial cds. | 429 | 93 |
| 701 | gi7020678 | Homo sapiens | cDNA FLJ20517 fis, clone KAT10235. | 2821 | 99 |
| 701 | gi10177966 | Arabidopsis thaliana | uridine kinase-like protein | 1068 | 44 |
| 701 | gi496728 | Saccharomyce s cerevisiae | uridine kinase | 775 | 37 |
| 702 | gi7022789 | Homo sapiens | cDNA FLJ10634 fis, clone NT2RP2005654, weakly similar to CYSTEINE STRING PROTEIN. | 1512 | 100 |
| 702 | AAB67446 | Homo sapiens | Amino acid sequence of a human | 1512 | 100 |

| SEQ ID | Accession | Species | Description | Score | % |
|--------|------------|---------------------------|---|-------|----------|
| NO: | No. | | | | Identity |
| | | | chaperone polypeptide. | 100 | |
| 702 | AAG01952 | Homo sapiens | Human secreted protein, SEQ ID NO: 6033. | 422 | 98 |
| 703 | gi7021321 | Homo sapiens | Gemin4 mRNA, complete cds. | 5481 | 99 |
| 703 | gi10945430 | Homo sapiens | chromosome 17 clone PAC P579 HC90, HC71AC, HC6 and HC56 genes, complete sequence. | 5452 | 100 |
| 703 | gi7018412 | Homo sapiens | mRNA; cDNA DKFZp434D174 (from clone DKFZp434D174). | 4359 | 99 |
| 704 | gi9964287 | Homo sapiens | hypertension-related calcium-regulated gene mRNA, complete cds. | 1129 | 100 |
| 704 | gi10434820 | Homo sapiens | cDNA FLJ13008 fis, clone NT2RP3000456. | 1129 | 100 |
| 704 | gi12803673 | Homo sapiens | , HT002 protein; hypertension-related calcium-regulated gene, clone MGC:3418, mRNA, complete cds. | 1129 | 100 |
| 705 | gi10435947 | Homo sapiens | cDNA FLJ13814 fis, clone THYRO1000368. | 3588 | 99 |
| 705 | gi3878402 | Caenorhabditis elegans | similar to C2 domain | 300 | 25 |
| 705 | gi3002479 | Leishmania major | L3162.1 | 198 | 25 |
| 706 | gi11907998 | Homo sapiens | BCL-6 corepressor (BCOR) mRNA, complete cds; alternatively spliced. | 2449 | 100 |
| 706 | gi7020277 | Homo sapiens | cDNA FLJ20285 fis, clone HEP04260. | 1131 | 99 |
| 706 | gi10432606 | Homo sapiens | cDNA FLJ11362 fis, clone HEMBA1000244. | 458 | 50 |
| 707 | gi7768662 | Homo sapiens | C4ST mRNA for chondroitin 4- sulfotranseferase, complete cds. | 1870 | 100 |
| 707 | gi8925966 | Homo sapiens | chondroitin 4-O-sulfotransferase 1 mRNA, complete cds. | 1870 | 100 |
| 707 | gi7572958 | Homo sapiens | mRNA for chondroitin-4-sulfotransferase (C4ST gene). | 1865 | 99 |
| 708 | gi2731561 | Homo sapiens | ATP receptor subunit (P2X5) mRNA, complete cds. | 2167 | 96 |
| 708 | gi1552522 | Homo sapiens | Human ionotropic ATP receptor P2X5a mRNA, complete cds. | 2131 | 96 |
| 708 | gi3387944 | Homo sapiens | clone 24793 ionotropic ATP receptor P2X5b mRNA, complete cds. | 1608 | 99 |
| 709 | gi7021105 | Homo sapiens | cDNA FLJ20793 fis, clone COL00343. | 1587 | 100 |
| 709 | gi7206854 | Caenorhabditis elegans | contains similarity to Pfam family PF00085 (Thioredoxins), Score 113, E=9.6e-33, N=1 | 435 | 29 |
| 709 | gi13775331 | Caenorhabditis elegans | contains similarity to Pfam family PF00085 (Thioredoxin), score=320.7, E=1.8e-95, N=3 | 297 | 28 |
| 710 | AAY04315 | Homo sapiens | Human secreted protein encoded by gene 23. | 385 | 100 |
| 710 | AAB12155 | Homo sapiens | Hydrophobic domain protein isolated from HT-1080 cells. | 385 | 100 |
| 711 | gi13624098 | Homo sapiens | cervical cancer 1 protooncogene protein p40 mRNA, complete cds. | 520 | 100 |
| 711 | gi12653253 | Homo sapiens | , DKFZP586A011 protein, clone MGC:8483, mRNA, complete cds. | 520 | 100 |
| 711 | gi4886473 | Homo sapiens | mRNA; cDNA DKFZp586A011 (from clone DKFZp586A011); partial cds. | 520 | 100 |
| 712 | gi927415 | Homo sapiens | H.sapiens mRNA for carnitine acetyltransferase. | 3209 | 98 |
| 712 | gi13879380 | Mus musculus | Similar to carnitine acetyltransferase | 3010 | 90 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|-------------------------------|--|-------|---------------|
| 712 | gi758632 | Mus musculus | carnitine acetyltransferase | 2967 | 89 |
| 713 | gi9437507 | Homo sapiens | TERA | 1198 | 100 |
| 713 | gi10439906 | Homo sapiens | cDNA: FLJ23279 fis, clone HEP06870. | 1198 | 100 |
| 713 | gi12652565 | Homo sapiens | , TERA protein, clone MGC:1093, mRNA, complete cds. | 1198 | 100 |
| 714 | gi7023336 | Homo sapiens | cDNA FLJ10964 fis, clone PLACE1000748. | 1196 | 100 |
| 714 | gi14198104 | Homo sapiens | , clone MGC:16981, mRNA, complete cds. | 1196 | 100 |
| 714 | gi7023823 | Homo sapiens | cDNA FLJ11269 fis, clone PLACE1009190. | 661 | 100 |
| 715 | AAB67579 | Homo sapiens | Amino acid sequence of a human hydrolytic enzyme HYENZ11. | 2740 | 100 |
| 715 | gi7020019 | Homo sapiens | cDNA FLJ20125 fis, clone COL06152. | 1973 | 99 |
| 715 | gi13527857 | Drosophila melanogaster | pol polyprotein | 298 | 26 |
| 716 | gi2218077 | Homo sapiens | gravin mRNA, complete cds. | 8920 | 99 |
| 716 | AAW53863 | Homo sapiens | Human gravin polypeptide. | 8868 | 99 |
| 716 | AAB15380 | Homo sapiens | Human gravin protein sequence. | 8868 | 99 |
| 717 | gi7021891 | Homo sapiens | cDNA FLJ10060 fis, clone HEMBA1001407. | 2306 | 99 |
| 717 | gi10433215 | Homo sapiens | cDNA FLJ11856 fis, clone HEMBA1006789. | 1959 | 86 |
| 717 | gi14042890 | Homo sapiens | cDNA FLJ14982 fis, clone Y79AA1000258. | 1959 | 86 |
| 718 | gi6224691 | Homo sapiens | Na+/sulfate cotransporter SUT-1 (SUT-1) mRNA, complete cds. | 3271 | 100 |
| 718 | AAB36158 | Homo sapiens | Novel human transporter protein SEQ ID NO: 2. | 3268 | 99 |
| 718 | AAB23625 | Homo sapiens | Human secreted protein SEQ ID NO: 50. | 3268 | 99 |
| 719 | gi7020123 | Homo sapiens | cDNA FLJ20189 fis, clone COLF0657. | 1264 | 99 |
| 719 | gi14328904 | Homo sapiens | fetal globin-inducing factor (FGIF) mRNA, complete cds. | 1262 | 99 |
| 719 | AAB71861 | Homo sapiens | Human FGIF. | 1262 | 99 |
| 720 | gi6690250 | Homo sapiens | clone HQ0659 PRO0659 mRNA, complete cds. | 926 . | 100 |
| 720 | gi12654109 | Homo sapiens | , PRO0659 protein, clone MGC:4888, mRNA, complete cds. | 926 | 100 |
| 721 | gi608025 | Homo sapiens | Human ankyrin G (ANK-3) mRNA, complete cds. | 580 | 32 |
| 721 | gi3885972 | Rattus norvegicus | 270 kDa ankyrin G isoform | 575 | 32 |
| 721 | gi178646 | Homo sapiens | Human erythroid ankyrin mRNA, complete cds. | 609 | 35 |
| 722 | gi7020915 | Homo sapiens | cDNA FLJ20666 fis, clone KAlA608. | 1229 | 96 |
| 722 | gi3169096 | Schizosacchar omyces pombe | possible pre-mRNA processing by similarity to yeast prp39 | 420 | 37 |
| 722 | gi1458279 | Caenorhabditis elegans | contains similarity to TPR domains | 252 | 29 |
| 723 | gi7020729 | Homo sapiens | cDNA FLJ20548 fis, clone KAT11542. | 2200 | 100 |
| 723 | gi10434720 | Homo sapiens | cDNA FLJ12942 fis, clone NTZRP2005139, weakly similar to 2-5A- DEPENDENT RIBONUCLEASE (EC 3.1.26-). | 2200 | 100 |
| 723 | gi11967781 | Homo sapiens | ANKRD2 gene for skeletal muscle ankyrin repeat, exons 1-9. | 174 | 30 |
| 724 | gi10433458 | Homo sapiens | cDNA FLJ12068 fis, clone HEMBB1002329. | 2903 | 99 |
| | | | cDNA FLJ12690 fis, clone | | 99 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|-------------------------------|--|-------|---------------|
| | | | NT2RM4002567. | | |
| 724 | gi10436665 | Homo sapiens | cDNA FLJ14252 fis, clone OVARC1001341. | 2167 | 99 |
| 725 | gi10434638 | Homo sapiens | cDNA FLJ12889 fis, clone NT2RP2004098, weakly similar to ADENYLATE CYCLASE (EC 4.6.1.1). | 3026 | 100 |
| 725 | gi14250313 | Homo sapiens | , clone MGC:16864, mRNA, complete cds. | 3026 | 100 |
| 725 | gi7020356 | Homo sapiens | cDNA FLJ20331 fis, clone HEP10410. | 1914 | 99 |
| 726 | AAY13947 | Homo sapiens | Human transmembrane protein, HP10495. | 655 | 100 |
| 726 | AAY07878 | Homo sapiens | Human secreted protein fragment encoded from gene 27. | 655 | 100 |
| 726 | gi6841296 | Homo sapiens | HSPC323 | 449 | 85 |
| 727 | gi7159733 | Homo sapiens | mRNA for ETAA16 protein. | 4318 | 100 |
| 727 | AAB10622 | Homo sapiens | Human Ewing tumor associated antigen protein. | 4318 | 100 |
| 728 | gi7020138 | Homo sapiens | cDNA FLJ20199 fis, clone COLF1162. | 2123 | 99 |
| 728 | AAY91948 | Homo sapiens | Human cytoskeleton associated protein 3 (CYSKP-3). | 1650 | 99 |
| 728 | gi7020210 | Homo sapiens | cDNA FLJ20246 fis, clone COLF6458. | 1474 | 99 |
| 729 | gi13182775 | Homo sapiens | CDA11 mRNA, complete cds. | 1495 | 99 |
| 729 | gi13937914 | Homo sapiens | , clone MGC:12519, mRNA, complete cds. | 973 | 97 |
| 729 | gi2257524 | Schizosacchar omyces pombe | HYPOTHETICAL 47.4KD PROTEIN IN SHP1-SEC17 INTERGENIC REGION | 536 | 42 |
| 730 | gi7020242 | Homo sapiens | cDNA FLJ20265 fis, clone COLF9334. | 2813 | 99 |
| 730 | gi14042159 | Homo sapiens | cDNA FLJ14559 fis, clone NT2RM2001998. | 2812 | 99 |
| 730 | gi499005 | Saccharomyce s cerevisiae | HRC830 | 128 | 32 |
| 731 | gi7022375 | Homo sapiens | cDNA FLJ10379 fis, clone NT2RM2002014. | 3182 | 99 |
| 731 | gi14010930 | Homo sapiens | BAC clone RP11-576F1 from 2, complete sequence. | 1868 | 100 |
| 731 | gi1573555 | Haemophilus influenzae Rd | transcription accessory protein (tex) | 691 | 42 |
| 732 | gi10434409 | Homo sapiens | cDNA FLJ12737 fis, clone NT2RP2000337. | 1001 | 99 |
| 733 | gi7019597 | Homo sapiens | clone PAC 270M7 chromosome 21 map 21q11.2, complete sequence. | 5944 | 100 |
| 733 | gi7407669 | Homo sapiens | chromosome 21 PAC 30P13 map 21q11.2, complete sequence, containing gene for nuclear factor RIP140. | 5944 | 100 |
| 733 | gi7717256 | Homo sapiens | chromosome 21 segment HS21C007. | 5944 | 100 |
| 734 | gi7021956 | Homo sapiens | cDNA FLJ10103 fis, clone HEMBA1002495, weakly similar to LIGHT-MEDIATED DEVELOPMENT PROTEIN DET1. | 1415 | 100 |
| 734 | AAB64828 | Homo sapiens | Human secreted protein sequence encoded by gene 12 SEQ ID NO:114. | 869 | 99 |
| 734 | gi4038594 | Lycopersicon esculentum | tDET1 protein | 413 | 37 |
| 735 | gi6752405 | Streptococcus pneumoniae | PspA | 137 | 24 |
| 736 | gi5080758 | Homo sapiens | chromosome 19, BAC 331191 (CIT-B- 471f3), complete sequence. | 1486 | 55 |
| 736 | gi456269 | Mus musculus domesticus | zinc finger protein 30 | 1478 | 54 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|-------------------------------|--|-------|---------------|
| 736 | gi4567179 | Homo sapiens | chromosome 19, BAC 37295 (CIT-B- 21A4), complete sequence. | 1281 | 62 |
| 737 | gi7023220 | Homo sapiens | cDNA FLJ10893 fis, clone NT2RP4002791. | 4557 | 99 |
| 737 | gi14042072 | Homo sapiens | cDNA FLJ14507 fis, clone NT2RM1000399. | 4439 | 97 |
| 737 | gi7582296 | Homo sapiens | BM-012 | 1807 | 99 |
| 738 | gi11596985 | Homo sapiens | chromosome 14 clone RP11-361H10 map 14q24.3, complete sequence. | 1751 | 100 |
| 738 | gi7020945 | Homo sapiens | cDNA FLJ20689 fis, clone KAIA2890. | 1738 | 99 |
| 738 | gi6067151 | Homo sapiens | chromosome 14 BAC 98L12, complete sequence. | 1159 | 100 |
| 739 | gi6941888 | Homo sapiens | ubiquitin-specific processing protease (USP25) mRNA, complete cds. | 5638 | 99 |
| 739 | AAB31550 | Homo sapiens | A human ubiquitin specific protease (USP). | 5638 | 99 |
| 739 | gi6693824 | Homo sapiens | ubiquitin-specific protease (USP21) mRNA, complete cds. | 4022 | 99 |
| 740 | gi6693824 | Homo sapiens | ubiquitin-specific protease (USP21) mRNA, complete cds. | 5465 | 99 |
| 740 | AAB31546 | Homo sapiens | A human ubiquitin specific protease 25 (USP25). | 5465 | 99 |
| 740 | AAF24881_ aa1 | Homo sapiens | DNA encoding a human ubiquitin specific protease 25 (USP25). | 5465 | 99 |
| 741 | gi7161175 | Homo sapiens | mRNA for 19A24 protein (19A24 gene). | 1726 | 100 |
| 741 | gi13021810 | Homo sapiens | NK cell receptor (CS1) mRNA, complete cds. | 1349 | 100 |
| 741 | AAB32373 | Homo sapiens | Human secreted protein sequence encoded by gene 3 SEQ ID NO:59. | 1349 | 100 |
| 742 | gi7023747 | Homo sapiens | cDNA FLJ11219 fis, clone PLACE1008122. | 2553 | 100 |
| 742 | gi7022222 | Homo sapiens | cDNA FLJ10287 fis, clone HEMBB1001387. | 880 | 97 |
| 742 | AAG01392 | Homo sapiens | Human secreted protein, SEQ ID NO: 5473. | 569 | 99 |
| 743 | gi7023747 | Homo sapiens | cDNA FLJ11219 fis, clone PLACE1008122. | 2442 | 97 |
| 743 | gi7022222 | Homo sapiens | cDNA FLJ10287 fis, clone HEMBB1001387. | 769 | 89 |
| 743 | AAG01392 | Homo sapiens | Human secreted protein, SEQ ID NO: 5473. | 569 | 99 |
| 744 | gi6434857 | Homo sapiens | pallid mRNA, complete cds. | 872 | 100 |
| 744 | gi13435969 | Homo sapiens | , pallid (mouse) homolog, pallidin, clone MGC:4983, mRNA, complete cds. | 872 | 100 |
| 744 | gi6456870 | Mus musculus | syntaxin 13-interacting protein pallid | 754 | 87 |
| 745 | gi6841480 | Homo sapiens | HSPC129 | 2378 | 99 |
| 745 | gi6841354 | Homo sapiens | HSPC058 cDNA FLJ10523 fis, clone | 1825 | 99 |
| 745 | gi7022613 | Homo sapiens | NT2RP2000863. | | 99 |
| 746 | gi7023644 | Homo sapiens | cDNA FLJ11155 fis, clone PLACE1006935. | 1826 | |
| 746 | AAB18981 | Homo sapiens | Amino acid sequence of a human transmembrane protein. | 1000 | 99 |
| 746 | gi13384531 | Caenorhabditis elegans | similar to C. elegans protein T16H12.10 | 680 | 40 |
| 747 | gi13544089 | Homo sapiens | , clone IMAGE:4053618, mRNA, partial cds. | 2749 | 99 |
| 747 | gi6007859 | Chlamydomon as reinhardtii | dynein heavy chain alpha | 246 | 30 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|-------------------------------|---|-------|---------------|
| 747 | gi2065436 | Schizosacchar omyces pombe | tealp | 227 | 28 |
| 748 | gi6650778 | Homo sapiens | PRO1575 | 297 | 100 |
| 749 | gi8926849 | Homo sapiens | mRNA for Pex3p, complete cds. | 1892 | 99 |
| 749 | gi4092648 | Homo sapiens | mRNA for PEX3 protein, partial. | 1892 | 99 |
| 749 | gi4218426 | Homo sapiens | pex3 gene (joined CDS, promoter and exon 1). | 1892 | 99 |
| 750 | gi309209 | Mus musculus | early B-cell factor | 3064 | 99 |
| 750 | gi6630994 | Homo sapiens | early B-cell transcription factor (EBF) mRNA, partial cds. | 3033 | 98 |
| 750 | gi7687988 | Gallus gallus | early B-cell factor | 3023 | 97 |
| 751 | gi10436636 | Homo sapiens | cDNA FLJ14228 fis, clone NT2RP3004148. | 3102 | 99 |
| 751 | gi14278861 | Homo sapiens | PHD zinc finger transcription factor mRNA, complete cds. | 2127 | 100 |
| 751 | gi12804495 | Homo sapiens | , clone IMAGE:3356959, mRNA, partial cds. | 1472 | 100 - |
| 752 | gi6594639 | Homo sapiens | dynein intermediate chain DNAII (DNAII) mRNA, complete cds. | 1773 | 100 |
| 752 | gi6635422 | Homo sapiens | dynein intermediate chain DNAI1 (DNAI1) gene, exon 20 and complete cds. | 1768 | 99 |
| 752 | gi927637 | Anthocidaris crassispina | dynein intermediate chain 2 | 961 | 61 |
| 753 | gi5924385 | Rattus norvegicus | ribosomal protein S271 | 412 | 100 |
| 753 | gi12803647 | Homo sapiens | , ribosomal protein S27 (metallopanstimulin 1), clone MGC:3659, mRNA, complete cds. | 412 | 100 |
| 753 | gi1373421 | Homo sapiens | Human ribosomal protein S27 mRNA, complete cds. | 412 | 100 |
| 754 | gi1655432 | Mus musculus | plexin 2 | 9646 | 96 |
| 754 | gi6010215 | Homo sapiens | mRNA for partial OCT/plexin-A2 protein. | 6985 | 99 |
| 754 | gi1665757 | Mus musculus | plexin 1 | 6359 | 63 |
| 755 | gi7770189 | Homo sapiens | PRO2325 | 901 | 100 |
| 756 | gi7022885 | Homo sapiens | cDNA FLJ10697 fis, clone NT2RP3000527, weakly similar to ZINC FINGER PROTEIN 43. | 3318 | 99 |
| 756 | gi10434872 | Homo sapiens | cDNA FLJ13043 fis, clone NT2RP3001338, weakly similar to ZINC FINGER PROTEIN 81. | 957 | 43 |
| 756 | gi38032 | Homo sapiens | Human ZNF43 mRNA. | 346 | 25 |
| 757 | gi14042238 | Homo sapiens | cDNA FLJ14604 fis, clone NT2RP1000363, moderately similar to R.norvegicus LL5 mRNA. | 1107 | 93 |
| 757 | AAB43723 | Homo sapiens | Human cancer associated protein sequence SEQ ID NO:1168. | 647 | 86 |
| 757 | gi14044043 | Homo sapiens | , clone IMAGE:4299555, mRNA, partial cds. | 467 | 66 |
| 758 | gi7106766 | Homo sapiens | HSPC188 | 532 | 100 |
| 758 | gi12804349 | Homo sapiens | , clone MGC:4355, mRNA, complete cds. | 529 | 99 |
| 758 | gi1002516 | Saccharomyce s cerevisiae | Hghlp | 115 | 27 |
| 759 | gi6175593 | Homo sapiens | transcription factor IIIC90 mRNA, complete cds. | 4326 | 99 |
| 760 | gi7023345 | Homo sapiens | cDNA FLJ10970 fis, clone PLACE1000948. | 647 | 99 |
| 760 | AAG03409 | Homo sapiens | Human secreted protein, SEQ ID NO: | 239 | 100 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|---------------------------|--|-------|---------------|
| | | | 7490. | | |
| 761 | gi5441541 | Canis familiaris | Ribosomal protein | 447 | 94 |
| 761 | gi304526 | Cricetulus griseus | ribosomal protein S17 | 447 | 94 |
| 761 | gi10439453 | Homo sapiens | cDNA: FLJ22917 fis, clone KAT06430. | 447 | 94 |
| 762 | gi6635353 | Homo sapiens | RUI (RUI) mRNA, complete cds. | 4638 | 99 |
| 762 | gi8100079 | Mus musculus | polycomb-group proteins | 4176 | 88 |
| 762 | gi8100077 | Rattus norvegicus | polycomb-group protein | 4152 | 88 |
| 763 | gi12804681 | Homo sapiens | , S100 calcium-binding protein, beta (neural), clone MGC:1323, mRNA, complete cds. | 479 | 100 |
| 763 | gi337730 | Homo sapiens | Human S100 protein beta-subunit gene, exon 3. | 479 | 100 |
| 763 | gi404769 | Mus musculus | S100 beta protein | 473 | 98 |
| 764 | gi7106782 | Homo sapiens | HSPC196 | 617 | 98 |
| 764 | gi7106786 | Homo sapiens | HSPC198 | 617 | 98 |
| 764 | AAW74871 | Homo sapiens | Human secreted protein encoded by gene 143 clone HBMDM46. | | 1 |
| 765 | gi3851206 | Homo sapiens | chromosome 19, cosmid F19847, complete sequence. | 1282 | 100 |
| 765 | gi13276629 | Homo sapiens | mRNA; cDNA DKFZp761D221 (from clone DKFZp761D221); complete cds. | 815 | 35 |
| 765 | gi5701573 | Caenorhabditis elegans | similar to S. pombe phosphoprotein (GB:X86179) | 430 | 33 |
| 766 | gi7020238 | Homo sapiens | cDNA FLJ20262 fis, clone COLF7748. | 1393 | 100 |
| 766 | gi12653607 | Homo sapiens | , clone IMAGE:3162218, mRNA, partial cds. | 1019 | 98 |
| 766 | AAY86358 | Homo sapiens | Human gene 11-encoded protein fragment, SEQ ID NO:273. | 996 | 95 |
| 767 | gi2588619 | Homo sapiens | BAC clone CTB-104F4 from 7q21-q22, complete sequence. | 2037 | 100 |
| 767 | gi1707507 | Homo sapiens | H.sapiens mRNA for mitochondrial transcription termination factor. | 2037 | 100 |
| 767 | gi12654289 | Homo sapiens | , transcription termination factor, mitochondrial, clone MGC:5000, mRNA, complete cds. | 2033 | 99 |
| 768 | gi1314373 | Homo sapiens | Human aquaporin-5 (AQP5) gene, exon 4 and complete cds. | 1336 | 100 |
| 768 | gi664760 | Rattus norvegicus | aquaporin-5 | 1245 | 91 |
| 768 | gi4894460 | Mus musculus | aquaporin 5 | 1235 | 91 |
| 769 | gi13097624 | Homo sapiens | , clone IMAGE:3608084, mRNA, partial cds. | 1093 | 100 |
| 769 | gi10438279 | Homo sapiens | cDNA: FLJ22029 fis, clone HEP08661. | 615 | 60 |
| 769 | gi13325154 | Homo sapiens | , clone IMAGE:3635709, mRNA, partial cds. | 609 | 45 |
| 770 | AAB48789 | Homo sapiens | Human prostate cancer-predisposing protein, CA7 CG04. | 2878 | 100 |
| 770 | gi11321424 | Mus musculus | Ral-A exchange factor RalGPS2 | 2073 | 96 |
| 770 | gi7637906 | Homo sapiens | Ral guanine nucleotide exchange factor RalGPS1A mRNA, complete cds. | 1224 | 70 |
| 771 | gi13623239 | Homo sapiens | , Similar to SGC32445 protein, clone MGC:10610, mRNA, complete cds. | 1080 | 99 |
| 771 | gi7547035 | Homo sapiens | SGC32445 protein (SGC32445) mRNA, complete cds. | 687 | 100 |
| 771 · | gi10434977 | Homo sapiens | cDNA FLJ13110 fis, clone NT2RP3002549, moderately similar to | 519 | 64 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|----------------------------------|---|-------|---------------|
| | | | HYPOTHETICAL 26.6 KD PROTEIN T19C3.4 IN CHROMOSOME III. | | |
| 772 | gi13939858 | Homo sapiens | RITA | 2614 | 100 |
| 772 | gi10048470 | Homo sapiens | C2H2-like zinc finger protein (ZNF463) mRNA, complete cds. | 2614 | 100 |
| 772 | gi8575775 | Homo sapiens | KRAB zinc finger protein (RITA) mRNA, complete cds. | 2614 | 100 |
| 773 | gi12654989 | Homo sapiens | , clone MGC:5623, mRNA, complete cds. | 2300 | 100 |
| 773 | gi3329425 | Homo sapiens | huntingtin interacting protein HYPE mRNA, partial cds. | 963 | 100 |
| 773 | gi429189 | Haemophilus somnus | surface protein | 152 | 41 |
| 774 | gi14028017 | Mesorhizobiu m loti | argininosuccinate lyase | 199 | 26 |
| 774 | gi2182606 | Rhizobium sp. NGR234 | Y4rH | 179 | 29 |
| 775 | gi3098311 | Oryctolagus cuniculus | elongation factor 1 A2 | 2410 | 100 |
| 775 | gi8886507 | Homo sapiens | elongation factor I A-2 (EF1A-2) gene, complete cds. | 2410 | 100 |
| 775 | gi12653327 | Homo sapiens | , eukaryotic translation elongation factor l alpha 2, clone MGC:8362, mRNA, complete cds. | 2410 | 100 |
| 776 | gi6624095 | Homo sapiens | BAC clone RP11-294L11 from 2, complete sequence. | 2515 | 97 |
| 776 | AAY66674 | Homo sapiens | Membrane-bound protein PRO1277. | 2515 | 97 |
| 776 | AAB87542 | Homo sapiens | Human PRO1277. | 2515 | 97 |
| 777 | gi6049162 | Homo sapiens | rhabdoid tumor deletion region protein 1 (RTDR1) mRNA, complete cds. | 1732 | 100 |
| 777 | gi14290442 | Homo sapiens | , rhabdoid tumor deletion region protein 1, clone MGC:16968, mRNA, complete cds. | 1732 | 100 |
| 778 | AAB66071 | Homo sapiens | Human INTERCEPT 296. | 1787 | 99 |
| 778 | AAB18992 | Homo sapiens | Amino acid sequence of a human transmembrane protein. | 880 | 58 |
| 778 | AAB26325 | Homo sapiens | Human CASB618 protein. | 880 | 58 |
| 779 | gi643656 | Rattus norvegicus | synaptotagmin VII | 1851 | 95 |
| 779 | gi12667446 | Rattus norvegicus | synaptotagmin VIIs | 1851 | 95 |
| 779 | gi6136786 | Mus musculus | synaptotagmin VII | 1842 | 95 |
| 780 | gi7020988 | Homo sapiens | cDNA FLJ20716 fis, clone HEP19742. | 1048 | 100 |
| 780 | gi4033606 | Adiantum capillus- veneris | Extensin | 131 | 38 |
| 780 | gi169347 | Phaseolus vulgaris | hydroxyproline-rich glycoprotein | 130 | 38 |
| 781 | gi7020477 | Homo sapiens | cDNA FLJ20401 fis, clone KAT00901. | 1644 | 96 |
| 781 | gi7022002 | Homo sapiens | cDNA FLJ10135 fis, clone HEMBA1003117. | 590 | 40 |
| 781 | gi7022284 | Homo sapiens | cDNA FLJ10324 fis, clone NT2RM2000567. | 590 | 40 |
| 782 | gi6808186 | Homo sapiens | mRNA; cDNA DKFZp434D0218 (from clone DKFZp434D0218); partial cds. | 1322 | 99 |
| 783 | gi505544 | Homo sapiens | H.sapiens mRNA for Zinc-finger protein (ZNFpT1). | 1211 | 99 |
| 783 | AAY58627 | Homo sapiens | Protein regulating gene expression PRGE-20. | 688 | 50 |
| 783 | gi9187356 | Homo sapiens | mRNA full length insert cDNA clone | 687 | 50 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|----------------------|--|-------|---------------|
| 110. | 1.0. | | EUROIMAGE 2107395. | | Lucitud |
| 784 | gi8896094 | Homo sapiens | SH3-containing protein SH3GLB2 mRNA, complete cds. | 1975 | 97 |
| 784 | gi4929591 | Homo sapiens | CGI-61 protein mRNA, complete cds. | 706 | 69 |
| 784 | gi8896092 | Homo sapiens | SH3-containing protein SH3GLB1 mRNA, complete cds. | 706 | 69 |
| 785 | gi7770175 | Homo sapiens | PRO2249 | 1827 | 99 |
| 785 | gi11527602 | Homo sapiens | mRNA for MCM10 homolog, complete cds. | 1827 | 99 |
| 785 | gi12053187 | Homo sapiens | mRNA; cDNA DKFZp434H152 (from clone DKFZp434H152); complete cds. | 1682 | 99 |
| 786 | gi7023364 | Homo sapiens | cDNA FLJ10982 fis, clone PLACE1001692, moderately similar to S- ACYL FATTY ACID SYNTHASE THIOESTERASE, MEDIUM CHAIN (EC 3.1.2.14). | 1413 | 99 |
| 786 | gi7023563 | Homo sapiens | cDNA FLJ11106 fis, clone PLACE1005763, moderately similar to S- ACYL FATTY ACID SYNTHASE THIOESTERASE, MEDIUM CHAIN (EC 3.1.2.14). | 1099 | 98 |
| 786 | gi205326 | Rattus norvegicus | S-acyl fatty acid sunthetase thio ester hydrolase, medium chain | -807 | 55 |
| 787 | gi2599502 | Homo sapiens | protocadherin 68 (PCH68) mRNA, complete cds. | 327 | 43 |
| 787 | AAY24913 | Homo sapiens | Human ontherin. | 327 | 43 |
| 787 | AAY94991 | Homo sapiens | Human secreted protein vc35_1, SEQ ID NO:22. | 296 | 28 |
| 788 | gi7023688 | Homo sapiens | cDNA FLJ11183 fis, clone PLACE1007488, weakly similar to PUTATIVE RHO/RAC GUANINE NUCLEOTIDE EXCHANGE FACTOR. | 2260 | 100 |
| 788 | gi3342246 | Rattus norvegicus | actin-filament binding protein Frabin | 725 | 32 |
| 788 | gi595425 | Homo sapiens | Human faciogenital dysplasia (FGD1) mRNA, complete cds. | 759 | 32 |
| 789 | gi6554165 | Homo sapiens | receptor protein tyrosine phosphatase (RPTP-rho) mRNA, alternatively spliced, complete cds. | 7734 | 99 |
| 789 | gi13378306 | Mus musculus | brain RPTPmam4 isoform I | 7499 | 97 |
| 789 | gi32456 | Homo sapiens | H.sapiens hR-PTPu gene for protein tyrosine phosphatase. | 4995 | 64 |
| 790 | gi7020479 | Homo sapiens | cDNA FLJ20402 fis, clone KAT00919. | 2024 | 99 |
| 790 | gi7770205 | Homo sapiens | PRO2521 | 1957 | 97 |
| 790 | gi10241843 | Mus musculus | gasdermin . | 282 | 29 |
| 791 | gi5262472 | Homo sapiens | mRNA; cDNA DKFZp564J102 (from clone DKFZp564J102); partial cds. | 1602 | 100 |
| 792 | gi10436457 | Homo sapiens | cDNA FLJ14084 fis, clone HEMBB1002383. | 830 | 100 |
| 792 | AAY94940 | Homo sapiens | Human secreted protein clone yi62_1 protein sequence SEQ ID NO:86. | 830 | 100 |
| 792 | AAY57922 | Homo sapiens | Human transmembrane protein HTMPN- 46. | 830 | 100 |
| 793 | gi7328061 | Homo sapiens | mRNA; cDNA DKFZp761I2312 (from clone DKFZp761I2312); partial cds. | 2723 | 100 |
| 793 | gi14039825 | Mus musculus | gamma-1 syntrophin | 2579 | 93 |
| 793 | gi8247279 | Homo sapiens | mRNA for syntrophin 4. | 2271 | 97 |
| 794 | gi6164674 | Homo sapiens | heterogeneous nuclear ribonucleoprotein, alternate transcript (RALY) mRNA, | 730 | 66 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|-------------------------|---------------------|---|--------------|---------------|
| NO: | 140. | | complete cds. | | Identity |
| 794 | gi14250048 | Homo sapiens | , heterogeneous nuclear ribonucleoprotein C (C1/C2), clone MGC:14574, mRNA, complete cds. | 705 | 53 |
| 794 | gi13937888 | Homo sapiens | , Similar to heterogeneous nuclear ribonucleoprotein C, clone MGC:12469, mRNA, complete cds. | 704 | 53 |
| 795 | gi12653905 | Homo sapiens | , Similar to Max dimerization protein 3, clone MGC:2383, mRNA, complete cds. | 1045 | 100 |
| 795 | AAY93137 | Homo sapiens | Human Myx protein. | 1023 | 98 |
| 795 | AAB35713 | Homo sapiens | Human Mad3 protein sequence. | 1010 | 97 |
| 796 | gi7020704 | Homo sapiens | cDNA FLJ20533 fis, clone KAT10931. | 585 | 98 |
| 797 | gi7106878 | Homo sapiens | HSPC244 | 398 | 98 |
| 797 | AAY07855 | Homo sapiens | Human secreted protein fragment encoded from gene 4. | 398 | 98 |
| 797 | gi13274582 | Mus musculus | thymus atrophy-related protein | 383 | 95 |
| 798 | gi8886483 | Gallus gallus | EURL | 1178 | 74 |
| 798 | gi10435877 | Homo sapiens | cDNA FLJ13763 fis, clone PLACE4000089. | 873 | 98 |
| 798 | AAG01108 | Homo sapiens | Human secreted protein, SEQ ID NO: 5189. | 561 | 100 |
| 799 | AAY33297 | Homo sapiens | Human membrane spanning protein MSP-4. | .781 | 100 |
| 799 | AAB61149 | Homo sapiens | Human NOV18 protein. | 781 | 100 |
| 799 | AAB61150 | Homo sapiens | Human NOV19 protein. | 781 | 100 |
| 800 | gi8099348 | Homo sapiens | zinc finger protein (ZFP) mRNA, complete cds. | 4066 | 99 |
| 800 | gi2293535 | Homo sapiens | zinc finger protein (ZnF20) mRNA, complete cds. | 1863 | 49 |
| 800 | gi11527849 | Mus musculus | zinc finger protein SKAT2 | 1323 | 58 |
| 801 | gi7023523 | Homo sapiens | cDNA FLJ11082 fis, clone PLACE1005206. | 2693 | 99 |
| 801 | gi9558010 | Leishmania major | possible cDNA flj11082 fis, clone place1005206 | 134 | 26 |
| 802 | gi6841558 | Homo sapiens | HSPC168 | 1502 | 100 |
| 802 | gi6453346 | Homo sapiens | Novel human gene on chromosome 20. | 1502 | 100 |
| 802 | gi13542748 | Mus musculus | RIKEN cDNA 3230401D17 gene | 1314 | 86 |
| 803 | gi7020468 | Homo sapiens | cDNA FLJ20396 fis, clone KAT00561. | 931 | 100 |
| 803 | AAB18980 | Homo sapiens | Amino acid sequence of a human transmembrane protein. | 931 | 100 |
| 803 | AAY91632 | Homo sapiens | Human secreted protein sequence encoded by gene 25 SEQ ID NO:305. | 914 | 98 |
| 804 | gi6650345 | Homo sapiens | alpha-catenin-like protein VR22 mRNA, complete cds. | 4478 | 99 |
| 804 | gi222788 | Gallus gallus | alpha N-catenin | 2765 | 60 |
| 804 | AAR58778 | Homo sapiens | Neural alpha-catenin protein. | 2765 | 60 |
| 805 . | gi10434911 | Homo sapiens | cDNA FLJ13068 fis, clone NT2RP3001739, weakly similar to HYPOTHETICAL 72.5 KD PROTEIN C2F7.10 IN CHROMOSOME I. | 587 | 38 |
| 805 | gi5912258 | Homo sapiens | mRNA; cDNA DKFZp586K0524 (from clone DKFZp586K0524); partial cds. | 190 | 41 |
| 805 | gi7022673 | Homo sapiens | cDNA FLJ10562 fis, clone NT2RP2002701. | 154 | 44 |
| | | Homo sapiens | cDNA FLJ13763 fis, clone | 876 | 99 |
| 806 | gi 1043 5877 | riolio sapiens | PLACE4000089. | | l |
| 806 806 | gi10435877 gi8886483 | Gallus gallus | | 868 | 72 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|-------------------------------|--|-------|---------------|
| 807 | gi4521254 | Mus musculus | cornichon-like protein | 867 | 100 |
| 807 | AAB60464 | Homo sapiens | Human cell cycle and proliferation protein CCYPR-12, SEQ ID NO:12. | 729 | 81 |
| 807 | AAY76218 | Homo sapiens | Human secreted protein encoded by gene 95. | 716 | 81 |
| 808 | gi7407144 | Homo sapiens | protocadherin Fat 2 (FAT2) mRNA, complete cds. | 22667 | 99 |
| 808 | gi3449286 | Rattus norvegicus | MEGF1 | 18806 | 81 |
| 808 | gi6688786 | Mus musculus | mouse fat 1 cadherin | 8928 | 47 |
| 809 | gi7407144 | Homo sapiens | protocadherin Fat 2 (FAT2) mRNA, complete cds. | 19770 | 99 |
| 809 | gi3449286 | Rattus norvegicus | MEGF1 · | 16567 | 82 |
| 809 | gi6688786 | Mus musculus | mouse fat 1 cadherin | 8928 | 47 |
| 810 | gi7020201 | Homo sapiens | cDNA FLJ20241 fis, clone COLF6335. | 2420 | 100 |
| 810 | gi10435321 | Homo sapiens | cDNA FLJ13337 fis, clone OVARC1001880. | 1279 | 99 |
| 810 | gi7020600 | Homo sapiens | cDNA FLJ20475 fis, clone KAT07206. | 634 | 60 |
| 811 | gi6483290 | Homo sapiens | CDH7 mRNA for cadherin-7, complete cds. | 4032 | 100 |
| 811 | gi10803408 | Homo sapiens | mRNA for cadherin-7 (CDH7 gene). | 3965 | 98 |
| 811 | gi868001 | Gallus gallus | chicken cadherin-7 | 3830 | 93 |
| 812 | gi13276621 | Homo sapiens | mRNA; cDNA DKFZp761G1913 (from clone DKFZp761G1913). | 1204 | 97 |
| 812 | gi8977983 | Mus musculus | neuronal interacting factor X I (NIX1) | 699 | 78 |
| 812 | gi10437116 | Homo sapiens | cDNA: FLJ21097 fis, clone CAS03931. | 297 | 42 |
| 814 | gi13279269 | Homo sapiens | , clone IMAGE:3631943, mRNA, partial cds. | 1480 | 100 |
| 814 | gi6808028 | Homo sapiens | mRNA; cDNA DKFZp761C029 (from clone DKFZp761C029); partial cds. | 857 | 100 |
| 814 | AAW88657 | Homo sapiens | Secreted protein encoded by gene 124 clone HPMCJ92. | 436 | 94 |
| 815 | gi7959853 | Homo sapiens | PRO1966 | 281 | 100 |
| 816 | gi7259234 | Mus musculus | contains transmembrane (TM) region | 718 | 65 |
| 816 | AAY94954 | Homo sapiens | Human secreted protein clone iw66_1 protein sequence SEQ ID NO:114. | 679 | 58 |
| 816 | AAB62810 | Homo sapiens | Human nervous system associated protein NSPRT3 amino acid sequence. | 678 | 61 |
| 817 | gi5921144 | Schizosacchar omyces pombe | mip1 | 1489 | 48 |
| 817 | gi458938 | Saccharomyce s cerevisiae | Yhr186cp | 469 | 30 |
| 817 | gi9366720 | Trypanosoma brucei | possible t16o11.22 protein. | 277 | 45 |
| 819 | gi7020799 | Homo sapiens | cDNA FLJ20590 fis, clone KAT09052. | 727 | 100 |
| 820 | gi7020555 | Homo sapiens | cDNA FLJ20449 fis, clone KAT05575. | 1857 | 99 |
| 820 | AAY79269 | Homo sapiens | Human testis-specific transcription factor PHELIX. | 1696 | 99 |
| 821 | gi6482350 | Homo sapiens | CAC-1 mRNA, partial cds. | 1136 | 100 |
| 821 | gi13937595 | Homo sapiens | , Similar to RIKEN cDNA 1810017F10 gene, clone MGC:2583, mRNA, complete cds. | 560 | 94 |
| 821 | AAY25770 | Homo sapiens | Human secreted protein encoded from gene 60. | 560 | 94 |
| 822 | gi10434608 | Homo sapiens | cDNA FLJ12871 fis, clone NT2RP2003751. | 2023 | 100 |
| 822 | gi6093227 | Homo sapiens | mRNA; cDNA DKFZp434I0850 (from clone DKFZp434I0850); partial cds. | 1607 | 100 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|--------------------------------|--|-------|---------------|
| 822 | gi6453452 | Homo sapiens | mRNA; cDNA DKFZp434L0850 (from clone DKFZp434L0850). | 1607 | 100 |
| 823 | AAY13402 | Homo sapiens | Amino acid sequence of protein PRO310. | 1079 | 63 |
| 823 | AAB18988 | Homo sapiens | Amino acid sequence of a human transmembrane protein. | 1079 | 63 |
| 823 | AAB80270 | Homo sapiens | Human PRO310 protein. | 1079 | 63 |
| 824 | gi13938181 | Homo sapiens | , clone IMAGE:2905978, mRNA, partial cds. | 2722 | 99 |
| 824 | gi6453540 | Homo sapiens | mRNA; cDNA DKFZp434D0428 (from clone DKFZp434D0428); partial cds. | 2455 | 99 |
| 824 | gi10440436 | Homo sapiens | mRNA for FLJ00053 protein, partial cds. | 807 | 100 |
| 825 | gi7022318 | Homo sapiens | cDNA FLJ10346 fis, clone NT2RM2001004. | 1475 | 100 |
| 826 | gi7110152 | Mus musculus | selenocysteine lyase SCLY | 1219 | 80 |
| 826 | gi7022600 | Homo sapiens | cDNA FLJ10515 fis, clone NT2RP2000764, weakly similar to NIFS PROTEIN. | 592 | 98 |
| 826 | gi9887215 | Methanosarcin a thermophila | cysteine desulfurase NifS | 315 | 43 |
| 827 | gi7022560 | Homo sapiens | cDNA FLJ10491 fis, clone NT2RP2000239. | 1266 | 100 |
| 827 | gi7022033 | Homo sapiens | cDNA FLJ10156 fis, clone HEMBA1003447. | 1161 | 97 |
| 828 | gi8247250 | Homo sapiens | mRNA for neutral sphingomyelinase II (nSMase2 gene). | 3489 | 100 |
| 828 | AAB70772 | Homo sapiens | Human neutral cerebral sphingomyelinase protein. | 3489 | 100 |
| 828 | gi8247281 | Mus musculus | neutral sphingomyelinase II | 3187 | 91 |
| 829 | gi7020945 | Homo sapiens | cDNA FLJ20689 fis, clone KAIA2890. | 2459 | 100 |
| 829 | gi11596985 | Homo sapiens | chromosome 14 clone RP11-361H10 map 14q24.3, complete sequence. | 1819 | 97 |
| 829 | gi6067151 | Homo sapiens | chromosome 14 BAC 98L12, complete sequence. | 1153 | 99 |
| 830 | gi10039443 | Homo sapiens | NEDL1 mRNA for NEDD4-like ubiquitin ligase 1, complete cds. | 4335 | 56 |
| 830 | AAW93167 | Homo sapiens | Human ZGGBP1 protein. | 992 | 47 |
| 830 | gi1374782 | Mus musculus | possible ubiquitin protein ligase | 1062 | 50 |
| 831 | gi7021974 | Homo sapiens | cDNA FLJ10115 fis, clone HEMBA1002777. | 1882 | 99 |
| 831 | gi7021027 | Homo sapiens | cDNA FLJ20739 fis, clone HEP07341. | 1252 | 98 |
| 831 | gi5002381 | Takifugu rubripes | BAW | 776 | 72 |
| 832 | gi7022523 | Homo sapiens | cDNA FLJ10469 fis, clone NT2RP2000008, weakly similar to ZINC FINGER PROTEIN 84. | 3772 | 99 |
| 832 | gi1020145 | Homo sapiens | Human DNA binding protein (HPF2) mRNA, complete cds. | 1714 | 48 |
| 832 | gi7243633 | Homo sapiens | RB-associated KRAB repressor (RBAK) mRNA, complete cds. | 1653 | 46 |
| 833 | gi6433864 | Homo sapiens | CLDN12 gene for claudin-12. | 1295 | 100 |
| 833 | gi12053057 | Homo sapiens | mRNA; cDNA DKFZp434I1816 (from clone DKFZp434I1816); complete cds. | 1295 | 100 |
| 833 | gi9799020 | Mus musculus | claudin-12 | 1125 | 91 |
| 834 | gi12053151 | Homo sapiens | mRNA; cDNA DKFZp434G0326 (from clone DKFZp434G0326); complete cds. | 5605 | 99 |
| 834 | gi7020102 | Homo sapiens | cDNA FLJ20176 fis, clone COL09928. | 1268 | 88 |
| 834 | gi7023725 | Homo sapiens | cDNA FLJ11205 fis, clone PLACE1007843. | 719 | 100 |
| 835 | gi7020789 | Homo sapiens | cDNA FLJ20583 fis, clone KAT09685. | 2153 | 99 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % |
|---------------|------------------|---------------------------|--|-------|----------------|
| 835 | AAG02503 | Homo sapiens | Human secreted protein, SEQ ID NO: 6584. | 423 | Identity 98 |
| 835 | gi14289183 | Homo sapiens | chac mRNA for chorein, complete cds. | 193 | 24 |
| 836 | gi7022600 | Homo sapiens | cDNA FLJ10515 fis, clone NT2RP2000764, weakly similar to NIFS PROTEIN. | 1301 | 100 |
| 836 | gi7110152 | Mus musculus | selenocysteine lyase SCLY | 1107 | 83 |
| 836 | gi13592392 | Caenorhabditis elegans | Contains similarity to Pfam domain: PF00266 (aminotran_5), Score=51.6, E- value=5.7e-12, N=1 | 468 | 44 |
| 837 | gi7274380 | Homo sapiens | group III secreted phospholipase A2 mRNA, complete cds. | 2813 | 99 |
| 837 | gi4314431 | Homo sapiens | PAC clone RP3-412A9 from 22, complete sequence. | 596 | 99 |
| 837 | gi5627 | Apis mellifera | phospholipase A-2 | 243 | 41 |
| | gi8331760 | Homo sapiens | X28 region near ALD locus containing dual specificity phosphatase 9 (DUSP9), ribosomal protein L18a (RPL18a), Ca2+/Calmodulin-dependent protein (Kinase I (CAMKI), creatine transporter (CRTR), CDM protein (CDM), adrenoleukodystrophy protein (ALD), plexin-related protein (PLXB3), musclespecific serine kinase (MSSK), NADisocitrate dehydrogenase (IDH), translocon-associated protein delta (TRAP), and LUI protein (LUI) genes, complete eds; and CCp pseudogene, complete sequence. | 3242 | 100 |
| 838 | gi6651019 | Mus musculus | semaphorin cytoplasmic domain- associated protein 3A | 1583 | 50 |
| 838 | gi6651021 | Mus musculus | semaphorin cytoplasmic domain- associated protein 3B | 1583 | 50 |
| 839 | gi7023290 | Homo sapiens | cDNA FLJ10932 fis, clone OVARC1000588. | 718 | 100 |
| 840 | gi6094681 | Homo sapiens | PAC clone RP5-1049N15 from 7q31.2- 7q32, complete sequence. | 4804 | 100 |
| 840 | gi7264724 | Homo sapiens | alpha-aminoadipate semialdehyde synthase mRNA, complete cds. | 4804 | 100 |
| 840 | gi4938304 | Homo sapiens | mRNA for lysine-ketoglutarate reductase/saccharopine dehydrogenase, partial CDS. | 4799 | 99 |
| 841 | AAY66700 | Homo sapiens | Membrane-bound protein PRO1137. | 1164 | 95 |
| 841 | AAB65223 | Homo sapiens | Human PRO1137 (UNQ575) protein sequence SEQ ID NO:250. | 1164 | 95 |
| 841 | AAY50917 | Homo sapiens | Human fetal brain cDNA clone vc4_1 derived protein. | 1023 | 100 |
| 842 | AAW56477 | Homo sapiens | Amino acid sequence of human bone morphogenetic protein-16 (BMP-16). | 1183 | 100 |
| 842 | AAY03849 | Homo sapiens | Human nodal protein. | 1183 | 100 |
| 842 | gi296605 | Mus musculus | nodal | 986 | 84 |
| 843 | gi7020399 | Homo sapiens | cDNA FLJ20356 fis, clone HEP15821. | 5470 | 100 |
| 843 | gi10435659 | Homo sapiens | cDNA FLJ13605 fis, clone PLACE1010562. | 224 | 44 |
| 844 | gi4886471 | Homo sapiens | mRNA; cDNA DKFZp586N0819 (from clone DKFZp586N0819). | 531 | 100 |
| 845 | gi3288470 | Homo sapiens | surf5c mRNA, clone 10.9. | 728 | 100 |
| 845 | gi3288452 | Homo sapiens | Surf-5 and Surf-6 genes. | 334 | 94 |
| 845 | gi3288468 | Homo sapiens | surf5b mRNA, clone L5. | 334 | 94 |
| 846 | . gi14149050 | Drosophila | turtle protein, isoform 4 | 1037 | 32 |

| SEQ ID | Accession | Species | Description | Score | % |
|------------|------------------------|---------------------------|---|-------------|----------|
| NO: | No. | melanogaster | | | Identity |
| 846 | gi14149048 | Drosophila | turtle protein, isoform 3 | 1037 | 32 |
| 640 | g114149048 | melanogaster | turtie protein, isotorin 5 | 1037 | 32 |
| 846 | gi14149046 | Drosophila | turtle protein, isoform 2 | 939 | 34 |
| | - | melanogaster | | | |
| 847 | gi7021049 | Homo sapiens | cDNA FLJ20753 fis, clone HEP02714. | 2930 | 99 |
| 847 | gi9886896 | Human | Orf73 | 175 | 20 |
| | | herpesvirus 8 | | | ļ |
| 847 | gi11037008 | Human herpesvirus 8 | latent nuclear antigen | 172 | 20 |
| 848 | gi12597293 | Homo sapiens | acidic mammalian chitinase precursor, | 2018 | 100 |
| 848 | gi6467177 | Homo sapiens | mRNA, complete cds. TSA1902-L mRNA for novel member of | 2010 | 99 |
| 848 | g1646/1// | Homo sapiens | chitinase family, complete cds. | 2010 | 99 |
| 848 | gi6467179 | Homo sapiens | TSA1902-S mRNA for novel member of | 1725 | 99 |
| 0.0 | g10407172 | Tionio sapiens | chitinase family, complete cds. | 1723 | " |
| 849 | gi32391 | Homo sapiens | Human HOX4C mRNA for a homeobox | 1802 | 98 |
| | | | protein. | | 1 |
| 849 | gi51416 | Mus musculus | Hox-4.4 | 1591 | 88 |
| 849 | gi4322104 | Danio rerio | homeobox protein | 425 | 82 |
| 850 | gi1359443 | Homo sapiens | Human gene for hepatitis C-associated | 2299 | 99 |
| | | | microtubular aggregate protein p44, exon | | |
| | I | <u> </u> | 9 and complete cds. | 2222 | l |
| 850 | AAY05371 | Homo sapiens | Human HCMV inducible gene protein, | 2299 | 99 |
| 850 | gj218576 | Pan | SEQ ID NO 10. | 2242 | 97 |
| 650 | gi218370 | troglodytes | P ⁴⁻⁴ | 2242 | " |
| 851 | gi575494 | Homo sapiens | MHC class II lymphocyte antigen beta- | 437 | 72 |
| | 5 | | chain (HLA-DPB1a) mRNA, complete | | |
| | | | cds. | | 1 |
| 851 | gi188479 | Homo sapiens | Human MHC class II lymphocyte antigen | 437 | 72 |
| | | | (HLA-DP) beta chain mRNA, complete | | 1 |
| | | | cds. | | |
| 851 | gi14044082 | Homo sapiens | , Similar to major histocompatibility | 429 | 70 |
| | | | complex, class II, DP beta 1, clone MGC:14112, mRNA, complete cds. | 1 | i |
| 852 | gi181547 | Homo sapiens | defensin 6 mRNA, complete cds. | 318 | 90 |
| 852 | AAR44819 | Homo sapiens | Sequence of the gastrointestinal defensin | 318 | 90 |
| 052 | AARTTOIS | Tromo sapiens | (GID) peptide calledhuman defensin 6. | 3.0 | 170 |
| 852 | gi1200182 | Homo sapiens | Human defensin 6 (HD-6) gene, complete | 314 | 89 |
| | Ŭ. | | cds. | | 1 |
| 853 | gi13396914 | Homo sapiens | The gene of C2GnT3 | 2389 | 100 |
| 853 | gi7527464 | Homo sapiens | core 2 beta-1,6-N- | 2389 | 100 |
| | | | acetylglucosaminyltransferase 3 | | |
| 050 | 1 1710000 | | (C2GnT3) mRNA, complete cds. | 0000 | 100 |
| 853 | AAU00037 | Homo sapiens | Human C2GnT3. PRO1483 | 2389 252 | 100 |
| 855 856 | gi7959772 gi5911169 | Homo sapiens Homo sapiens | transmembrane mucin 12 (MUC12) | 2914 | 99 |
| 830 | gijelilee | Homo sapiens | mRNA, partial cds. | 2914 | 99 |
| 856 | AAY59290 | Homo sapiens | Human MUC12 polypeptide. | 2914 | 99 |
| 856 | gi2589172 | Rattus | mucin Muc3 | 595 | 36 |
| - | | norvegicus | | | 1 |
| 857 | AAE00508 | Homo sapiens | Human lipase protein, MLip-1. | 1456 | 100 |
| 857 | gi56600 | Rattus | triacylglycerol lipase | 776 | 58 |
| | | norvegicus | | | |
| 857 | gi3108175 | Mus musculus | pancreatic lipase related protein 1 | 772 | 57 |
| 858 | AAY94954 | Homo sapiens | Human secreted protein clone iw66_1 | 1112 | 100 |
| 0.50 | | | protein sequence SEQ ID NO:114. | 070 | 100 |
| 858 | gi10434269 | Homo sapiens | cDNA FLJ12650 fis, clone | 872 | 100 |

| SEQ ID | Accession No. | Species | Description | Score | % Identity |
|--------|------------------|----------------------------------|--|-------|---------------|
| NO: | NO. | | NT2RM4002054. | | lucitity |
| 858 | gi7259234 | Mus musculus | contains transmembrane (TM) region | 660 | 60 |
| 859 | gi7021851 | Homo sapiens | cDNA FLJ10035 fis, clone HEMBA1000919. | 1589 | 100 |
| 859 | gi10440420 | Homo sapiens | mRNA for FLJ00045 protein, partial cds. | 654 | 89 |
| 859 | AAY99671 | Homo sapiens | Human GTPase associated protein-22. | 654 | 89 |
| 860 | gi7022523 | Homo sapiens | cDNA FLJ10469 fis, clone NT2RP2000008, weakly similar to ZINC FINGER PROTEIN 84. | 3573 | 99 |
| 860 | gi1020145 | Homo sapiens | Human DNA binding protein (HPF2) mRNA, complete cds. | 1604 | 48 |
| 860 | gi12584159 | Homo sapiens | zinc finger protein 268 (ZNF268) mRNA, complete cds. | 1542 | 48 |
| 861 | gi6539434 | Homo sapiens | SPR1 mRNA, complete cds. | 808 | 100 |
| 861 | gi6523547 | Volvox carteri f. nagariensis | hydroxyproline-rich glycoprotein DZ- HRGP | 185 | 39 |
| 861 | gi904359 | Beta vulgaris | chitinase 1 | 185 | 41 |
| 862 | gi7021924 | Homo sapiens | cDNA FLJ10081 fis, clone HEMBA1002018. | 2742 | 100 |
| 862 | gi10435862 | Homo sapiens | cDNA FLJ13751 fis, clone PLACE3000339, weakly similar to GLUCOAMYLASE S1/S2 PRECURSOR (EC 3.2.1.3). | 2687 | 99 |
| 862 | gi11275988 | Homo sapiens | testis development protein PRTD mRNA, complete cds. | 2454 | 99 |
| 863 | gi7019913 | Homo sapiens | cDNA FLJ20060 fis, clone COL01358. | | 100 |
| 863 | gi10434817 | Homo sapiens | cDNA FLJ13006 fis, clone NT2RP3000449. | 1823 | .99 |
| 863 | gi10434659 | Homo sapiens | cDNA FLJ12902 fis, clone NT2RP2004347. | 1724 | 99 |
| 864 | gi7329718 | Homo sapiens | Novel human gene mapping to chomosome 1. | | 99 |
| 864 | gi7022765 | Homo sapiens | cDNA FLJ10619 fis, clone NT2RP2005472. | 3153 | 99 |
| 864 | gi14388939 | Homo sapiens | chorea-acanthocytosis (CHAC) mRNA, complete cds. | 462 | 30 |
| 865 | gi28971 | Homo sapiens | H.sapiens mRNA for autoantigen NOR- 90. | 3813 | 100 |
| 865 | gi509241 | Homo sapiens | Human mRNA for upstream binding factor (hUBF). | 2661 | 78 |
| 865 | AAB44430 | Homo sapiens | Human lung tumour-specific antigen encoded by cDNA | 2649 | 78 |
| 866 | gi13445482 | Homo sapiens | HP43.8KD mRNA, complete cds. | 282 | 47 |
| 866 | gi10434108 | Homo sapiens | cDNA FLJ12552 fis, clone NTZRM4000712, moderately similar to Homo sapiens ubiquitin hydrolyzing enzyme I (UBH1) mRNA. | | |
| 866 | gi10436670 | Homo sapiens | cDNA FLJ14256 fis, clone PLACE1000007, weakly similar to PROBABLE UBIQUITIN CARBOXYL- TERMINAL HYDROLASE R10E11.3 (EC 3.1.2.15). | 219 | 36 |
| . 867 | AAB73229 | Homo sapiens | Human phosphatase MTMR7_h. | 743 | 57 |
| 867 | gi5901814 | Drosophila melanogaster | BcDNA.GH04637 | 503 | 48 |
| 867 | . gi7020021 | Homo sapiens | cDNA FLJ20126 fis, clone COL06160. | 697 | 73 |
| 868 | gi7959801 | Homo sapiens | PRO0800 | 392 | 100 |
| 869 | gi 12654971 | Homo sapiens | , calcium-regulated heat-stable protein (24kD), clone MGC:5586, mRNA, | 417 | 97 |

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|-------------------------------|---|-------|---------------|
| | | | complete cds. | | |
| 869 | gi13097198 | Homo sapiens | , calcium-regulated heat-stable protein (24kD), clone MGC:5235, mRNA, complete cds. | 417 | 97 |
| 869 | AAW61023 | Homo sapiens | Human RNA binding protein. | 417 | 97 |
| 870 | gi6650832 | Homo sapiens | PRO2086 | 243 | 100 |
| 871 | gi2217942 | Rattus norvegicus | glycoprotein specific UDP- glucuronyltransferase | 1802 | 97 |
| 871 | gi8051678 | Homo sapiens | hu-GlcAT-P mRNA for glucuronyltransferase, complete cds. | 1757 | 99 |
| 871 - | gi4519214 | Rattus norvegicus | UDP-glucuronyltransferase-S | 760 | 50 |
| 872 | gi14286288 | Homo sapiens | , Similar to RIKEN cDNA 2010004P11 gene, clone MGC:2734, mRNA, complete cds. | 715 | 100 |
| 872 | gi13529665 | Mus musculus | RIKEN cDNA 2010004P11 gene | 706 | 98 |
| 872 | gi2565364 | Musca domestica | Sex-lethal protein | 134 | 33 |
| 873 | gi190406 | Homo sapiens | Human profilaggrin gene exons 1-3, 5' end. | 6301 | 99 |
| 873 | gi190396 | Homo sapiens | Human profilaggrin gene, 3' end. | 5133 | 99 |
| 873 | gi190404 | Homo sapiens | Human profilaggrin mRNA, 3' end. | 3696 | 89 |
| 874 | gi791002 | Homo sapiens | ARSD gene, complete CDS. | 1761 | 99 |
| 874 | gi6651286 | Homo sapiens | arylsulfatase D beta (ARSD) mRNA, complete cds. | 1756 | 99 |
| 874 | gi791004 | Homo sapiens | ARSE gene, complete CDS. | 947 | 58 |
| 875 | gi13097675 | Homo sapiens | , Similar to uncharacterized hypothalamus protein HCDASE, clone MGC:1171, mRNA, complete cds. | 612 | 96 |
| 875 | AAY87599 | Homo sapiens | Human fatty acid beta-oxidation enzyme HUFA-2. | 612 | 96 |
| 875 | AAG03352 | Homo sapiens | Human secreted protein, SEQ ID NO: 7433. | 591 | 100 |
| 876 | gi6180180 | Homo sapiens | transcription factor IGHM enhancer 3, 1M11 protein, JM4 protein, JM5 protein, TS4 protein, JM10 protein, A4 differentiation-dependent protein, triple LIM domain protein 6, and synaptophysin genes, complete cds; and L-type calcium channel alpha-1 subunit gene, partial cds, complete sequence. | 908 | 100 |
| 876 | gi3114826 | Homo sapiens | mRNA for IM4 protein, complete CDS (clone IMAGE 546750 and LLNLc110F1857Q7 (RZPD Berlin)). | 908 | 100 |
| 876 | gi7673612 | Mus musculus | DXImx39e protein | 831 | 91 |
| 877 | gi13543663 | Homo sapiens | , ubiquitin-conjugating enzyme E2D 1 (homologous to yeast UBC4/5), clone MGC:14673, mRNA, complete cds. | 805 | 100 |
| 877 | gi460810 | Homo sapiens | H.sapiens UBCH5 mRNA for ubiquitin conjugating enzyme. | 805 | 100 |
| 877 | gi4868140 | Homo sapiens | ubiquitin-conjugating enzyme HBUCE1 mRNA, complete cds. | 747 | 91 |
| 878 | gi7020915 | Homo sapiens | cDNA FLJ20666 fis, clone KAIA608. | 1288 | 100 |
| 878 | gi3169096 | Schizosacchar omyces pombe | possible pre-mRNA processing by similarity to yeast prp39 | 279 | 33 |
| 878 | gi10177721 | Arabidopsis thaliana | gene_id:MPL12.20~ | 146 | 22 |
| 879 | gi7020681 | Homo sapiens | cDNA FLJ20519 fis, clone KAT10365. | 891 | 100 |
| 879 | AAY87267 | Homo sapiens | Human signal peptide containing protein | 824 | 95 |

WO 02/22660 PCT/US01/26015

| SEQ ID NO: | Accession No. | Species | Description | Score | % Identity |
|---------------|------------------|--------------------------|---|-------|---------------|
| | | | HSPP-44 SEQ ID NO:44. | | |
| 879 | AAB65245 | Homo sapiens | Human PRO1104 (UNQ547) protein sequence SEQ ID NO:297. | 824 | 95 |
| 880 | gi6560622 | Homo sapiens | PRO0611 | 501 | 100 |
| 881 | AAB57079 | Homo sapiens | Human prostate cancer antigen protein sequence SEQ ID NO:1657. | 668 | 100 |
| 881 | AAY99372 | Homo sapiens | Human PRO1430 (UNQ736) amino acid sequence SEQ ID NO:116. | 668 | 100 |
| 881 | AAB88356 | Homo sapiens | Human membrane or secretory protein clone PSEC0082. | 661 | 99 |
| 882 | gi1381181 | Oryctolagus cuniculus | ubiquitin-conjugating enzyme E2-32k | 663 | 100 |
| 882 | gi13436071 | Homo sapiens | , clone MGC:10481, mRNA, complete cds. | 663 | 100 |
| 882 | gi7020506 | Homo sapiens | cDNA FLJ20419 fis, clone KAT02435. | 658 | 99 |
| 883 | gi1381181 | Oryctolagus cuniculus | ubiquitin-conjugating enzyme E2-32k | 1265 | 99 |
| 883 | gi13436071 | Homo sapiens | , clone MGC:10481, mRNA, complete cds. | 1265 | 99 |
| 883 | gi7020506 | Homo sapiens | cDNA FLJ20419 fis, clone KAT02435. | 1256 | 98 |
| 884 | gi1381181 | Oryctolagus cuniculus | ubiquitin-conjugating enzyme E2-32k | 383 | 97 |
| 884 | gi13436071 | Homo sapiens | , clone MGC:10481, mRNA, complete cds. | 383 | 97 |
| 884 | gi7020506 | Homo sapiens | cDNA FLJ20419 fis, clone KAT02435. | 383 | 97 |
| 885 | gi14424536 | Homo sapiens | , Similar to septin 6, clone MGC:16619, mRNA, complete cds. | 2183 | 99 |
| 885 | gi5689158 | Mus musculus | Septin6 | 2114 | 95 |
| 885 | gi7023141 | Homo sapiens | cDNA FLJ10849 fis, clone NT2RP4001414, highly similar to SEPTIN 2 HOMOLOG. | 1840 | 82 |
| 886 | gi14424536 | Homo sapiens | , Similar to septin 6, clone MGC:16619, mRNA, complete cds. | 1213 | 63 |
| 886 | gi5689158 | Mus musculus | Septin6 | 1162 | 62 |
| 886 | gi7023141 | Homo sapiens | cDNA FLJ 10849 fis, clone NT2RP4001414, highly similar to SEPTIN 2 HOMOLOG. | 995 | 51 |
| 887 | gi4309951 | Homo sapiens | BAC clone RP11-121A8 from 7p14-p13, complete sequence. | 684 | 100 |
| 887 | AAG00417 | Homo sapiens | Human secreted protein, SEQ ID NO: 4498. | 684 | 100 |
| 887 | gi339159 | Homo sapiens | Human T-cell receptor germline gamma- chain gene V-region (V3; subgroup I). | 392 | 73 |
| 888 | gi2570015 | Homo sapiens | H.sapiens PAX7 gene, exon 1 (and joined CDS). | 2756 | 100 |
| 888 | gi2570021 | Homo sapiens | H.sapiens mRNA for paired box containing transcription factor, PAX7. | 2756 | 100 |
| 888 | gi2570014 | Homo sapiens | H.sapiens PAX7 gene, exon 1 (and joined CDS). | 2735 | 99 |

TABLE 3

| SEQ ID NO: | Accession No. | Description | Results* |
|---------------|------------------|---------------------------------------|------------------------------------|
| 445 | BL00434 | HSF-type DNA-binding domain proteins. | BL00434C 23.85 7.111e-09 1089-1129 |
| 446 | PD00066 | PROTEIN ZINC-FINGER | PD00066 13.92 1.000e-13 216-229 |
| | | METAL-BINDI. | PD00066 13.92 2.286e-12 244-257 |
| | | | PD00066 13.92 4.522e-11 299-312 |
| | 1 ' | | PD00066 13.92 6.538e-10 157-170 |
| | 1 | | PD00066 13.92 7.923e-10 327-340 |
| 453 | PR00037 | LACR BACTERIAL | PR00037A 12.66 6.786e-09 34-49 |
| | | REGULATORY PROTEIN | |
| | | HTH SIGNATURE | |
| 465 | PR00320 | G-PROTEIN BETA WD-40 | PR00320C 13.01 6.100e-09 197-212 |
| | | REPEAT SIGNATURE | PR00320C 13.01 6.400e-09 393-408 |
| | | 1 | PR00320A 16.74 8.683e-09 197-212 |
| | | | PR00320B 12.19 9.775e-09 299-314 |
| 466 | DM00215 | PROLINE-RICH PROTEIN | DM00215 19.43 5.881e-09 14-47 |
| | | 3. | |
| 470 | BL00175 | Phosphoglycerate mutase | BL00175D 27.67 8.500e-40 175-227 |
| | | family phosphohistidine | BL00175C 23.75 5.000e-25 90-122 |
| | ł | proteins. | BL00175A 15.42 8.333e-20 17-37 |
| | 1 | | BL00175B 12.60 1.000e-12 66-79 |
| 472 | BL00315 | Dehydrins proteins. | BL00315A 9.35 8.119e-09 105-133 |
| 473 | BL00518 | Zinc finger, C3HC4 type | BL00518 12.23 4.000e-11 44-53 |
| | | (RING finger), proteins. | |
| 475 | PD02448 | TRANSCRIPTION | PD02448A 9.37 4.293e-09 171-210 |
| | | PROTEIN DNA-BINDIN. | |
| 477 | PR00625 | DNAJ PROTEIN FAMILY | PR00625A 12.84 8.500e-19 121-141 |
| | ì | SIGNATURE | PR00625B 13.48 3.204e-15 151-172 |
| 478 | PD02102 | SUBUNIT E V-ATPASE | PD02102A 16.74 5.853e-10 26-70 |
| | l . | VACUOLAR ATP | |
| | | SYNTHASE HYDROL. | |
| 479 | BL00018 | EF-hand calcium-binding | BL00018 7.41 4.706e-11 49-62 |
| | | domain proteins. | |
| 480 | PR00501 | KELCH REPEAT | PR00501A 8.25 9.182e-09 544-558 |
| | | SIGNATURE | |
| 483 | PR00878 | CHOLINESTERASE | PR00878F 5.37 5.179e-12 500-513 |
| | | SIGNATURE | |
| 484 | BL00378 | Hexokinases proteins. | BL00378C 16.14 1.000e-40 207-251 |
| | | | BL00378E 22.92 1.000e-40 725-771 |
| | 1 | | BL00378C 16.14 3.520e-40 655-699 |
| | 1 | | BL00378E 22.92 3.382e-36 277-323 |
| | 1 | 1 | BL00378B 14.23 5.333e-35 509-546 |
| | 1 | 1 | BL00378B 14.23 8.953e-28 61-98 |
| | | 1 | BL00378A 19.01 1.346e-22 22-50 |
| | 1 | 1 | BL00378F 8.27 2.688e-17 893-908 |
| | 1 | | BL00378D 10.94 6.294e-17 703-715 |
| | 1 | 1 | BL00378D 10.94 5.500e-16 255-267 |
| | 1 | | BL00378F 8.27 9.609e-13 445-460 |
| | | | BL00378A 19.01 3.017e-12 470-498 |
| 485 | BL00028 | Zinc finger, C2H2 type, | BL00028 16.07 2.688e-15 352-369 |
| | | domain proteins. | BL00028 16.07 4.375e-15 324-341 |
| | | | BL00028 16.07 4.176e-14 604-621 |
| | | 1 | BL00028 16.07 8.412e-14 380-397 |
| | 1 | | BL00028 16.07 9.471e-14 576-593 |
| | 1 | | BL00028 16.07 1.450e-13 548-565 |
| | | | BL00028 16.07 2.350e-13 436-453 |
| | | | BL00028 16.07 4.150e-13 492-509 |
| | 1 | 1 | BL00028 16.07 5.050e-13 296-313 |
| | 1 | 1 | BL00028 16.07 1.783e-12 520-537 |

| SEQ ID | Accession | Description | Results* |
|--------|------------|--|--|
| NO: | No. | | BL00028 16.07 3.348e-12 632-649 |
| | • | 1 | BL00028 16.07 5.3486-12 032-049 BL00028 16.07 5.304e-12 408-425 |
| | | | BL00028 16.07 5.304e-12 408-425 |
| | | 1 | BL00028 16.07 4.808e-11 464-481 |
| | | | BL00028 16.07 7.000e-10 268-285 |
| 486 | BL00301 | GTP-binding elongation | BL00301B 20.09 1.429e-26 128-160 |
| | | factors proteins. | BL00301A 12.41 6.400e-15 62-74 |
| 487 | PD00301 | PROTEIN REPEAT | PD00301B 5.49 7.600e-12 826-837 |
| | | MUSCLE CALCIUM-BI. | |
| 489 | BL00227 | Tubulin subunits alpha, beta, | BL00227B 19.29 1.000e-40 52-107 |
| | | and gamma proteins. | BL00227C 25.48 1.000e-40 113-165 |
| | | • | BL00227D 18.46 1.000e-40 222-276 |
| | | | BL00227F 21.16 1.000e-40 382-436 |
| | | | BL00227E 24.15 6.727e-36 326-361 |
| | | | BL00227A 24.55 2.125e-33 1-35 |
| 490 | BL00479 | Phorbol esters / | BL00479B 12.57 6.625e-09 1271-1287 |
| | | diacylglycerol binding | |
| 401 | BL00479 | domain proteins. Phorbol esters / | BL00479B 12.57 6.625e-09 1250-1266 |
| 491 | BL00479 | diacylglycerol binding | BE00479B 12.37 0.0236-09 1230-1200 |
| | Į. | diacylgiycerol oliiding domain proteins. | |
| 492 | BL00107 | Protein kinases ATP-binding | BL00107A 18.39 5.500c-19 138-169 |
| 492 | BLUUIU | region proteins. | BL00107B 13.31 1.000e-16 203-219 |
| 493 | BL50002 | Src homology 3 (SH3) | BL50002A 14.19 5.000e-15 392-411 |
| 773 | DESCOOL | domain proteins profile. | BL50002B 15.18 2.500e-09 430-444 |
| 494 | PR00049 | WILM'S TUMOUR | PR00049D 0.00 6.949e-09 87-102 |
| | 1111111111 | PROTEIN SIGNATURE | |
| 497 | BL00914 | Syntaxin / epimorphin | BL00914 24.91 6.172e-09 249-299 |
| | | family proteins. | • |
| 498 | PD00066 | PROTEIN ZINC-FINGER | PD00066 13.92 8.200e-16 362-375 |
| | | METAL-BINDI. | PD00066 13.92 4.462c-15 334-347 |
| | 1 | | PD00066 13.92 8.615e-15 473-486 |
| | | | PD00066 13.92 5.200e-14 306-319 |
| | | | PD00066 13.92 3.000e-13 390-403 PF007801 14.69 7.863e-09 293-323 |
| 500 | PF00780 | Domain found in NIK1-like kinases, mouse citron and | PF00780114.69 7.863e-09 293-323 |
| | | yeast ROM. | |
| 501 | BL00518 | Zinc finger, C3HC4 type | BL00518 12.23 7.333e-09 279-288 |
| 301 | DECOSTS | (RING finger), proteins: | * |
| 502 | DM01418 | 352 FIBRILLAR | DM01418A 20.83 2.050e-23 1537-1585 |
| 302 | DIVIOLATO | COLLAGEN CARBOXYL- | DM01418B 22.51 5.895e-21 1632-1674 |
| | | TERMINAL. | DM01418C 20.48 8.571e-18 1702-1744 |
| 508 | BL01052 | Calponin family repeat | BL01052B 15.31 1.000e-09 131-157 |
| | 1 | proteins. | |
| 512 | BL01310 | ATP1G1/PLM/MAT8 | BL01310 14.74 7.107e-36 27-63 |
| | | family proteins. | |
| 515 | DM00475 | w LOW TRANSPOSASE | DM00475B 12.12 6.019e-09 386-406 |
| | | SAPA 12K. | |
| 516 | BL00636 | Nt-dnaJ domain proteins. | BL00636A 8.07 5.865e-11 64-81 |
| 519 | PR00625 | DNAJ PROTEIN FAMILY | PR00625A 12.84 2.019e-14 76-96 |
| | | SIGNATURE | PR00625B 13.48 5.714e-11 106-127 |
| 520 | BL00216 | Sugar transport proteins. | BL00216B 27.64 6.400e-10 92-142 |
| 523 | BL01033 | Globins profile. | BL01033B 13.81 1.000e-15 38-50 |
| 526 | BL50002 | Src homology 3 (SH3) | BL50002B 15.18 4.750e-12 1075-1089 |
| | Processe | domain proteins profile. | PR00249G 15.72 8.892e-10 387-409 |
| 531 | PR00249 | SECRETIN-LIKE GPCR SUPERFAMILY | PR00249G 15.72 8.892e-10 387-409 PR00249C 17.08 6.609e-09 223-247 |
| | | SUPERFAMILY | FRUUZ+7C 17.08 0.0098-09 223-247 |
| 532 | BL00528 | Ribosomal protein S4e | BL00528D 27.17 8.012e-09 341-395 |
| 352 | BL00528 | proteins. | BL00320D 21.11 8.0126-07 341-393 |
| | | | |

| SEQ ID NO: | Accession No. | Description | Results* |
|---------------|------------------|---|---|
| 534 | PR00194 | TROPOMYOSIN SIGNATURE | PR00194C 6.38 1.900e-35 109-138 PR00194E 8.74 1.000e-30 195-221 PR00194D 9.57 8.714e-27 139-163 PR00194B 10.24 2.800e-25 84-105 PR00194A 7.86 5.500e-22 48-66 |
| 535 | PR00194 | TROPOMYOSIN SIGNATURE | PR00194C 6.38 1.900e-35 109-138 PR00194E 8.74 1.000e-30 195-221 PR00194B 10.24 2.800e-25 84-105 PR00194D 9.57 1.900e-23 139-163 PR00194A 7.86 5.500e-22 48-66 |
| 538 | PR00019 | LEUCINE-RICH REPEAT SIGNATURE | PR00019A 11.19 5.050e-11 110-124 |
| 541 | BL00540 | Ferritin iron-binding regions proteins. | BL00540A 15.06 1.000e-40 32-73 BL00540B 18.82 1.000e-40 123-178 BL00540C 13.00 7.750e-14 188-200 |
| 546 | PR00153 | CYCLOPHILIN PEPTIDYL-PROLYL CIS- TRANS ISOMERASE SIGNATURE | PR00153E 9.10 2.385e-15 121-137 |
| 548 | BL00115 | Eukaryotic RNA polymerase II heptapeptide repeat proteins. | BL00115Z 3:12 8:213e-09 63-112 |
| 549 | BL01282 | BIR repeat proteins. | BL01282B 30.49 2.373e-12 317-356 |
| 551 | BL00570 | Bacterial ring hydroxylating dioxygenases alpha-subunit signa. | BL00570B 19.03 9.357e-09 277-309 |
| 553 | PD01427 | TRANSFERASE METHYLTRANSFERASE BI. | PD01427B 22.45 7.000e-11 127-168 |
| 554 | PR00048 | C2H2-TYPE ZINC FINGER SIGNATURE | PR00048A 10.52 7.632e-11 447-461 |
| 555 | PD02637 | SERUM PARAOXONASE/ARYLES TERASE P. | PD02637A 14.261.000e-40 32.87 PD02637G 13.821.000e-40 307.355 PD02637D 13.69 6.053e-36 170-218 PD02637B 10.33 8.875e-34 106-141 PD02637B 11.92 8.200e-28 218-249 PD02637C 7.53 3.520e-27 141-170 PD02637F 15.62 9.438e-26 281-307 |
| 556 | DM00892 | 3 RETROVIRAL PROTEINASE. | DM00892C 23.55 2.768e-16 474-508 |
| 557 | BL00039 | DEAD-box subfamily ATP- dependent helicases proteins. | BL00039D 21.67 5.179e-36 294-340 BL00039A 18.44 7.955e-29 15-54 BL00039C 15.63 1,300e-16 143-167 BL00039B 19.19 2.465e-12 58-84 |
| 558 | PR00507 | N12 CLASS N6 ADENINE- SPECIFIC DNA METHYLTRANSFERASE SIGNATURE | PR00507B 14.16 8.932e-09 83-98 |
| 559 | BL00383 | Tyrosine specific protein phosphatases proteins. | BL00383E 10.35 8.683e-12 242-253 |
| 566 | PD00066 | PROTEIN ZINC-FINGER METAL-BINDI. | PD00066 13.92 5.500e-13 214-227 |
| 572 | BL01160 | Kinesin light chain repeat proteins. | BL01160B 19.54 4.432e-09 76-130 |
| 573 | BL00422 | Granins proteins. | BL00422C 16.18 4.638e-10 49-77 |
| 574 | PR00319 | BETA G-PROTEIN (TRANSDUCIN) SIGNATURE | PR00319A 15.27 7.911e-10 452-469 PR00319A 15.27 2.180e-09 410-427 |
| 577 | BL00269 | Mammalian defensins proteins. | BL00269C 16.52 6.786e-26 73-102 BL00269A 8.53 2.607e-20 8-28 BL00269B |

| 000 10 | Accession | Description | Results* |
|---------------|-----------|---|---|
| SEQ ID NO: | No. | Description | Results |
| NO: | 140. | | 19.17 5.500e-17 35-64 |
| 578 | PD02327 | GLYCOPROTEIN | PD02327B 19.84 2.241e-11 157-179 |
| 376 | FD02327 | ANTIGEN PRECURSOR | 1 2023273 19:04 2:2410-11 157-179 |
| | | IMMUNOGLO. | • |
| 579 | BL00596 | High potential iron-sulfur | BL00596B 13.07 9.743e-09 273-285 |
| | | proteins. | |
| 580 | BL00915 | Phosphatidylinositol 3- and | BL00915C 22.43 8.147e-32 1015-1054 |
| | | 4-kinases proteins. | BL00915D 27.02 9.217e-27 1092-1128 |
| | | | BL00915B 22.78 3.382e-25 918-956 |
| | | | BL00915A 10.09 5.500e-10 756-768 |
| 584 | BL00038 | Myc-type, 'helix-loop-helix' | BL00038B 16.97 7.488e-09 499-520 |
| | | dimerization domain | |
| | | proteins. | TY 000000 10 00 00 00 100 510 |
| 585 | BL00795 | Involucrin proteins. | BL00795C 17.06 9.200e-09 498-543 BL00710 12.98 9.100e-17 159-174 |
| 586 | BL00710 | Phosphoglucomutase and phosphomannomutase | BL00/10 12.98 9.100e-1/ 139-1/4 |
| | | phosphoserine signa. | |
| 587 | BL00518 | Zinc finger, C3HC4 type | BL00518 12.23 5.714e-10 34-43 |
| 38/ | BLUUSIA | (RING finger), proteins. | BL00318 12.23 3.7146-10 34-43 |
| 588 | PR00326 | GTP1/OBG GTP-BINDING | PR00326A 8.75 5.979e-14 257-278 |
| 300 | 1 100320 | PROTEIN FAMILY | 110032011 0.73 3.5750 1 1 257 270 |
| | | SIGNATURE | |
| 591 | BL00548 | Ribosomal protein S3 | BL00548 20.58 7.000e-19 66-96 |
| | | proteins. | |
| 592 | BL00478 | LIM domain proteins. | BL00478B 14.79 1.250e-12 557-572 |
| | | | BL00478B 14.79 6.000e-12 494-509 |
| | | | BL00478B 14.79 2.400e-11 624-639 |
| 594 | PR00109 | TYROSINE KINASE | PR00109B 12.27 3.681e-13 141-160 |
| | | CATALYTIC DOMAIN | |
| | | SIGNATURE | PRO0040D 0 00 0 062 - 12 510 525 |
| 596 | PR00049 | WILM'S TUMOUR PROTEIN SIGNATURE | PR00049D 0.00 9.063e-12 510-525 PR00049D 0.00 8.286e-10 513-528 |
| | 1 | PROTEIN SIGNATURE | PR00049D 0.00 8.280e-10 513-528 |
| | | | PR00049D 0.00 9.429e-10 511-526 |
| 599 | BL00232 | Cadherins extracellular | BL00232B 32.79 4.750e-40 142-190 |
| 5,, | 2244252 | repeat proteins domain | BL00232A 27.72 3.793e-22 48-81 |
| | i | proteins. | BL00232B 32.79 1.257e-16 251-299 |
| | İ | | BL00232C 10.65 5.935e-14 249-267 |
| | | | BL00232D 16.25 3.368e-13 763-778 |
| | | | BL00232B 32.79 3.512e-11 366-414 |
| 600 | DM00215 | PROLINE-RICH PROTEIN | DM00215 19.43 9.695e-09 513-546 |
| | | 3. | PF00583B 10.18 9.100e-10 120-130 |
| 601 | PF00583 | Acetyltransferase (GNAT) | PF00583B 10.18 9.100e-10 120-150 |
| 602 | PR00326 | family. GTP1/OBG GTP-BINDING | PR00326A 8.75 5.950e-11 146-167 |
| 002 | PK00320 | PROTEIN FAMILY | FR00320A 6.73 3.5300-11 140-107 |
| | 1 | SIGNATURE | |
| 604 | BL00319 | Amyloidogenic glycoprotein | BL00319C 17.12 6.000e-10 136-170 |
| 004 | DECOSIO | extracellular domain | |
| | | proteins. | |
| 607 | BL00239 | Receptor tyrosine kinase | BL00239F 28.15 4.717e-25 477-522 |
| | | class II proteins. | BL00239E 17.14 5.897e-23 423-473 |
| | _ | | BL00239C 18.75 7.600e-17 372-395 |
| 608 | PD01066 | PROTEIN ZINC FINGER | PD01066 19.43 3.357e-32 10-49 |
| | | ZINC-FINGER METAL- | |
| | PRODUCE | BINDING NU. | DD 00440 + 12 20 4 808 - 10 5 27 |
| 609 | PR00449 | TRANSFORMING | PR00449A 13.20 4.808e-10 5-27 PR00449D 10.79 5.636e-09 111-125 |
| | | PROTEIN P21 RAS SIGNATURE | TRUU-123 10.75 3.0300-1311-123 |
| 610 | PF00791 | Domain present in ZO-1 and | PF00791C 20.98 2.412e-09 1-40 |
| 010 | T FF00/91 | Domain present in 20-1 and | 11007710 20.70 2.7120-07 1-40 |

| SEQ ID NO: | Accession No. | Description | Results* |
|---------------|------------------|--|---|
| 140: | 140. | Unc5-like netrin receptors. | |
| 612 | PR00109 | TYROSINE KINASE CATALYTIC DOMAIN SIGNATURE | PR00109B 12.27 9.234e-13 487-506 |
| 613 | BL00678 | Trp-Asp (WD) repeat proteins proteins. | BL00678 9.67 1.600e-10 104-115 BL00678 9.67 5.737e-09 62-73 BL00678 9.67 8.105e-09 146-157 BL00678 9.67 8.105e-09 276-287 |
| 615 | PR00334 | HMW KININOGEN SIGNATURE | PR00334B 8.69 5.230e-10 460-484 PR00334B 8.69 1.771e-09 464-488 PR00334B 8.69 2.886e-09 466-490 PR00334B 8.69 8.200e-09 458-482 |
| 617 | DM00215 | PROLINE-RICH PROTEIN 3. | DM00215 19.43 5.881e-09 66-99 |
| 618 | PF00084 | Sushi domain proteins (SCR repeat proteins. | PF00084B 9.45 7.188e-10 539-551 PF00084B 9.45 7.300e-09 600-612 |
| 619 | PR00169 | POTASSIUM CHANNEL SIGNATURE | PR00169A 16.77 4.316e-09 72-92 |
| 621 | BL00845 | CAP-Gly domain proteins. | BL00845 16.43 1.900e-25 321-346 BL00845 16.43 9.325e-22 443-468 |
| 622 | BL01002 | Translationally controlled tumor protein. | BL01002D 18.24 4.706e-26 143-171 BL01002C 21.97 6.143e-26 79-110 BL01002A 13.19 1.360e-24 1-24 BL01002B 7.39 3.118e-14 48-62 |
| 624 | PR00049 | WILM'S TUMOUR PROTEIN SIGNATURE | PR00049D 0.00 8.857e-10 1030-1045 |
| 627 | PR00011 | TYPE III EGF-LIKE SIGNATURE | PR00011A 14.06 4.822e-09 475-494 |
| 629 | PF00930 | Dipeptidyl peptidase IV (DPP IV) N-terminal region. | PF00930J 15.96 5.000e-15 656-684 PF00930J 8.78 6.045e-12 708-729 |
| 630 | PF00930 | Dipeptidyl peptidase IV (DPP IV) N-terminal region. | PF00930I 15.96 5.000e-15 598-626 PF00930J 8.78 6.045e-12 650-671 |
| 631 | BL00303 | S-100/ICaBP type calcium binding protein. | BL00303B 26.15 1.844e-10 365-402 |
| 632 | BL00114 | Phosphoribosyl pyrophosphate synthetase proteins. | BL00114A 17.22 1.000e-40 54-101 BL00114B 15.90 1.000e-40 107-153 BL00114D 21.45 1.000e-40 208-259 BL00114C 18.22 2.895e-34 167-202 BL00114E 14.48 3.647e-25 293-317 |
| 635 | BL00870 | Chaperonins clpA/B proteins. | BL00870F 8.73 4.833e-36 376-425 BL00870G 8.07 6.553e-27 436-470 BL00870E 17.62 3.333e-16 304-359 |
| 639 | BL00633 | Bromodomain proteins. | BL00633B 13.82 9.775e-13 237-262 BL00633B 13.82 4.750e-11 80-105 |
| 641 | BL00299 | Ubiquitin domain proteins. | BL00299 28.84 7.962e-17 47-99 |
| 642 | PD02102 | SUBUNIT E V-ATPASE VACUOLAR ATP SYNTHASE HYDROL. | PD02102A 16.74 4.176e-10 97-141 |
| 643 | PD02080 | T-CELL GLYCOPROTEIN CD8 CHAIN SURFACE ALPHA PRE. | PD02080D 15.22 6.557e-09 269-306 |
| 644 | BL01245 | RIO1/ZK632.3/MJ0444 family proteins. | BL01245F 18.75 7.805e-14 239-276 |
| 646 | BL00469 | Nucleoside diphosphate kinases proteins. | BL00469 22.22 1.000e-40 41-96 |
| 649 | PR00217 | 43 KD POSTSYNAPTIC PROTEIN SIGNATURE | PR00217C 10.91 5.945e-09 91-107 |
| 651 | PR00326 | GTPI/OBG GTP-BINDING PROTEIN FAMILY SIGNATURE | PR00326A 8.75 7.600e-11 629-650 |

| SEQ ID NO: | Accession No. | Description | Results* |
|---------------|------------------|--|--|
| 652 | DM00215 | PROLINE-RICH PROTEIN 3. | DM00215 19.43 8.322e-09 227-260 |
| 653 | PF01298 | Transferrin binding protein. | PF01298C 15.13 1.000e-08 413-440 |
| 658 | PR00443 | G-PROTEIN ALPHA SUBUNIT GROUP S SIGNATURE | PR00443A 15.16 9.451e-09 89-105 |
| 659 | BL00518 | Zinc finger, C3HC4 type (RING finger), proteins. | BL00518 12.23 5.714e-10 34-43 |
| 663 | BL00466 | TFIIS zinc ribbon domain proteins. | BL00466 25.88 1.000e-32 294-331 |
| 664 | PD00567 | PROTEIN RNA-BINDING RNA REPEAT HYD. | PD00567B 18.23 3.172e-10 411-425 |
| 665 | BL00030 | Eukaryotic RNA-binding region RNP-1 proteins. | BL00030A 14.39 7.882e-11 10-29 |
| 669 | PR00124 | ATP SYNTHASE C SUBUNIT SIGNATURE | PR00124A 8.81 8.347e-11 117-137 |
| 670 | PD01234 | PROTEIN NUCLEAR BROMODOMAIN TRANS. | PD01234B 15.53 2.500e-10 38-56 |
| 671 | BL00466 | TFIIS zinc ribbon domain proteins. | BL00466 25.88 1.000e-32 219-256 |
| 672 | BL01282 | B1R repeat proteins. | BL01282B 30.49 2.068e-12 298-337 |
| 673 | BL00455 | Putative AMP-binding domain proteins. | BL00455 13.31 4.176e-14 201-217 |
| 674 | BL01160 | Kinesin light chain repeat proteins. | BL01160B 19.54 8.703e-10 407-461 BL01160B 19.54 2.373e-09 414-468 |
| 675 | BL00518 | Zinc finger, C3HC4 type (RING finger), proteins. | BL00518 12.23 5.286e-10 326-335 |
| 676 | BL00518 | Zinc finger, C3HC4 type (RING finger), proteins. | BL00518 12.23 5.286e-10 335-344 |
| 682 | PR00761 | BINDIN PRECURSOR SIGNATURE | PR00761E 14.32 4.789e-09 499-518 |
| 691 | BL00415 | Synapsins proteins. | BL00415Q 2.23 2.885e-09 83-119 |
| 692 | PR00211 | GLUTELIN SIGNATURE | PR00211B 0.86 6.167e-09 115-136 PR00320C 13.01 7:300e-09 297-312 |
| 694 | PR00320 | G-PROTEIN BETA WD-40 REPEAT SIGNATURE | |
| 696 | PD02952 | KINASE TRANSFERASE CHOLINE PROTEIN MULTIGENE FAMI. | PD02952C 15.76 5.701e-16 263-293 PD02952B 15.57 7.242e-11 243-257 PD02952A 11.84 9.625e-09 131-159 |
| 697 | PD00066 | PROTEIN ZINC-FINGER METAL-BINDI. | PD00066 13.92 7.231e-15 504-517 PD00066 13.92 5.800e-14 220-233 PD00066 13.92 1.000e-11 248-261 PD00066 13.92 5.696e-11 333-346 PD00066 13.92 2.500e-09 361-374 |
| 698 · | PR00205 | CADHERIN SIGNATURE | PR00205B 11.39 6.571e-13 167-185 |
| 699 | PR00049 | WILM'S TUMOUR PROTEIN SIGNATURE | PR00049D 0.00 4.966e-09 50-65 PR00049D 0.00 9.237e-09 74-89 |
| 701 | PR00988 | URIDINE KINASE SIGNATURE | PR00988A 6.39 6.600e-15 98-116 PR00988C 13.64 5.605e-13 175-191 PR00988E 8.27 8.393e-13 245-257 PR00988D 5.95 8.250e-11 231-242 PR00988F 12.23 9.820e-11 267-281 PR00988B 11.60 2.317e-10 128-140 |
| 702 · | PR00625 | DNAJ PROTEIN FAMILY SIGNATURE | PR00625A 12.84 1.804e-13 22-42 PR00625B 13.48 5.821e-13 53-74 |
| 706 | PF00023 | Ank repeat proteins. | PF00023A 16.03 2.286e-09 209-225 |
| 708 | BL01212 | ATP P2X receptors proteins. | BL01212A 34.89 1.000e-40 43-96 BL01212E 24.87 1.000e-40 227-282 BL01212D 11.42 6.700e-25 185-209 BL01212D 11.86 2.800e-24 310-338 BL01212B 19.25 3.571e-21 129-154 |

| SEQ ID NO: | Accession No. | Description | Results* |
|---------------|------------------|------------------------------------|---|
| | | | BL012)2C 8.40 1.214e-14 162-173 BL01212F 10.12 4.774e-14 291-302 |
| 709 | BL00194 | Thioredoxin family proteins. | BL00194 12.16 3.455e-17 45-58 |
| 712 | BL00439 | Acyltransferases ChoActase | BL00439F 26.22 1.000e-40 418-471 |
| ,12 | DECOTO | / COT / CPT family | BL00439E 19.05 2.440e-24 320-349 |
| | | proteins. | BL00439B 16.82 1.000e-20 167-189 |
| | | protonio. | BL00439H 18.24 4.600e-20 566-592 |
| | | į. | BL00439A 9.40 1.237e-15 35-52 |
| | | | BL00439D 13.11 4.545e-15 272-290 |
| | | | BL00439C 13.53 1.730e-11 248-261 |
| | | | BL00439G 13.40 9.719e-11 513-524 |
| 716 | BL00412 | Neuromodulin (GAP-43) proteins. | BL00412D 16.54 8.990e-09 305-356 |
| 718 | BL01271 | Sodium:sulfate symporter | BL01271D 25.26 5.979e-32 537-592 |
| | | family proteins. | BL01271A 8.06 6.250e-18 131-151 |
| | | | BL01271C 13.62 7.750e-17 464-486 |
| | | | BL01271B 12.02 1.563e-16 269-294 |
| 719 | PF00023 | Ank repeat proteins. | PF00023B 14.20 2.500e-10 141-151 |
| | | | PF00023A 16.03 4.000e-10 112-128 |
| 721 | PF00023 | Ank repeat proteins. | PF00023A 16.03 1.750e-10 66-82 |
| | | | PF00023B 14.20 5.500e-09 161-171 |
| | | | PF00023A 16.03 8.714e-09 363-379 |
| 725 | PR00019 | LEUCINE-RICH REPEAT | PR00019B 11.36 1.500e-11 173-187 |
| | | SIGNATURE | PR00019A 11.19 2.800e-11 314-328 |
| | | | PR00019A 11.19 5.050e-11 176-190 |
| | | | PR00019B 11.36 3.520e-09 311-325 |
| | | | PR00019B 11.36 4.600e-09 541-555 |
| | | | PR00019B 11.36 5.320e-09 471-485 |
| | | | PR00019A 11.19 6.000e-09 544-558 |
| | | | PR00019B 11.36 8.200e-09 242-256 |
| 701 | PR00681 | RIBOSOMAL PROTEIN SI | PR00019B 11.36 9.640e-09 127-141 PR00681I 8.81 9.897e-09 600-619 |
| 731 | | SIGNATURE | |
| 736 | PD01066 | PROTEIN ZINC FINGER | PD01066 19.43 9.581e-31 8-47 |
| | | ZINC-FINGER METAL- | 1 |
| | | BINDING NU. | |
| 739 | BL00972 | Ubiquitin carboxyl-terminal | BL00972A 11.93 1.587e-13 170-188 |
| | | hydrolases family 2 proteins. | BL00972D 22.55 8.826e-11 590-615 |
| 740 | BL00972 | Ubiquitin carboxyl-terminal | BL00972A 11.93 1.587e-13 170-188 |
| | | hydrolases family 2 proteins. | BL00972D 22.55 8.826e-11 590-615 |
| 741 | DM01688 | 2 POLY-IG RECEPTOR. | DM01688G 16.45 6.936e-10 85-117 |
| 747 | PF00646 | F-box domain proteins. | PF00646A 14.37 6.625e-09 50-64 |
| 753 | BL01168 | Ribosomal protein S27e proteins. | BL01168 15.74 1.000e-40 20-75 |
| 756 | PD00066 | PROTEIN ZINC-FINGER | PD00066 13.92 6.885e-10 127-140 |
| | | METAL-BINDI. | |
| 757 | PD00301 | PROTEIN REPEAT | PD00301B 5.49 7.231e-09 1019-1030 |
| | | MUSCLE CALCIUM-B1. | |
| 761 | BL00712 | Ribosomal protein S17e | BL00712B 12.56 1.000e-40 28-66 |
| | | proteins. | BL00712A 6.23 8.855e-19 2-22 |
| 762 | PF00878 | Cation-independent | PF00878T 17.51 3.818e-09 799-826 |
| | 1 | mannose-6-phosphate | |
| | | receptor repeat proteins. | |
| 763 | BL00303 | S-100/ICaBP type calcium | BL00303A 21.77 9.526e-31 3-40 |
| | | binding protein. | BL00303B 26.15 5.737e-30 50-87 |
| 766 | BL00018 | EF-hand calcium-binding | BL00018 7.41 6.087e-09 237-250 |
| | | domain proteins. | |
| 768 | BL00221 | MIP family proteins. | BL00221D 12.33 6.143e-19 180-195 |
| | | | BL00221C 13.36 1.000e-14 135-152 |
| | 1 | -1 | BL00221E 8.47 3.739e-13 203-214 |

| SEQ ID | Accession | Description | Results* |
|--------|-----------|--|---|
| NO: | No. | | _ · |
| | | | BL00221B 10.22 1.750e-12 63-74 |
| | | | BL00221A 6.39 5.200e-12 16-27 |
| 769 | PF00992 | Troponin. | PF00992A 16.67 8.859e-10 214-249 |
| 770 | BL00720 | Guanine-nucleotide dissociation stimulators CDC25 family sign. | BL00720B 16.57 8.297e-15 136-160 |
| 771 | PR00883 | HIGH MOBILITY GROUP- LIKE NUCLEAR PROTEIN SIGNATURE | PR00883A 6.49 8.920e-09 191-205 |
| 772 | PD01066 | PROTEIN ZINC FINGER ZINC-FINGER METAL- BINDING NU. | PD01066 19.43 6.786e-32 8-47 |
| 775 | BL00301 | GTP-binding elongation factors proteins. | BL00301B 20.09 5.500e-31 90-122 BL00301C 11.73 8.200e-15 423-437 BL00301A 12.41 3.842e-13 9-21 |
| 776 | PR00453 | VON WILLEBRAND FACTOR TYPE A DOMAIN SIGNATURE | PR00453A 12.79 4.892e-12 325-343 PR00453B 14.65 1.614e-10 162-177 PR00453A 12.79 3.152e-10 123-141 |
| 779 | PR00399 | SYNAPTOTAGMIN SIGNATURE | PR00399A 9.52 1.730e-13 145-161 PR00399B 14.27 2.059e-13 160-174 PR00399C 12.27 3.24e-12 216-232 PR00399D 14.48 3.930e-10 236-247 PR00399B 14.27 1.915e-09 291-305 |
| 780 | BL00115 | Eukaryotic RNA polymerase II heptapeptide repeat proteins. | BL00115Z 3.12 8.395e-10 123-172 BL00115Z 3.12 4.375e-09 137-186 |
| 783 | PD00066 | PROTEIN ZINC-FINGER METAL-BINDI. | PD00066 13.92 8.800e-14 165-178 PD00066 13.92 8.800e-14 193-206 PD00066 13.92 5.286e-12 249-262 PD00066 13.92 8.269e-10 221-234 |
| 786 | PF00975 | Thioesterase domain proteins. | PF00975B 10.82 2.688e-12 90-104 |
| 788 | DM01970 | 0 kw ZK632.12 YDR313C ENDOSOMAL III. | DM01970B 8.60 9.833e-16 632-645 |
| 789 | BL00740 | MAM domain proteins. | BL00740B 19.76 5.378e-12 174-195 BL00740C 15.93 4.000e-11 684-695 |
| 793 | PD00289 | PROTEIN SH3 DOMAIN REPEAT PRESYNA. | PD00289 9.97 9.500e-12 102-116 |
| 795 | BL00038 | Myc-type, 'helix-loop-helix' dimerization domain proteins. | BL00038A 13.61 3.400e-09 66-82 |
| 800 | PD01066 | PROTEIN ZINC FINGER ZINC-FINGER METAL- BINDING NU. | PD01066 19.43 5.050e-15 233-272 |
| 804 | BL00663 | Vinculin family talin- binding region proteins. | BL00663G 24.17 L000e-40 364-414 BL00663K 21.52 9.816e-40 735-790 BL006631 27.27 4.447e-35 514-568 BL006631 20.67 9.118e-27 802-838 BL006631 20.67 9.118e-27 802-838 BL00663F 20.78 2.000e-25 292-333 BL00663F 27.08 2.000e-25 292-333 BL00663F 27.88 4.629-23 4436-489 BL00663C 22.59 2.853e-23 104-159 BL00663D 27.78 4.629e-23 42-96 BL00663D 124.77 3.789e-18 179-226 BL00663A 11.51 2.350e-15 18-39 BL00663A 21.19 9.56e-10 227-265 |
| 808 | PR00010 | TYPE II EGF-LIKE SIGNATURE | PR00010C 11.16 7.545e-10 3968-3979 |
| 809 | PR00010 | TYPE II EGF-LIKE SIGNATURE | PR00010C 11.16 7.545e-10 3882-3893 |

| SEQ ID NO: | Accession No. | Description | Results* |
|---------------|------------------|--|---|
| 810 | DM00215 | PROLINE-RICH PROTEIN 3. | DM00215 19.43 2.929e-10 163-196 |
| 811 | PR00205 · | CADHERIN SIGNATURE | PR00205B 11.39 9.182e-15 243-261 PR00205A 14.73 1.000e-12 168-184 PR00205C 13.65 1.783e-12 503-518 PR00205B 11.39 9.294e-11 463-481 |
| 813 | PR00456 | RIBOSOMAL PROTEIN P2 SIGNATURE | PR00456E 3.06 5.146e-11 313-328 PR00456E 3.06 5.146e-11 314-329 PR00456E 3.06 5.146e-11 315-330 PR00456E 3.06 7.938e-10 312-327 PR00456E 3.06 7.938e-10 316-331 |
| 818 | BL01071 | grpE protein. | BL01071A 24.88 8.277e-21 78-124 BL01071B 18.21 5.286e-15 195-219 |
| 826 | DM00813 | AMINOTRANSFERASES CLASS-V PYRIDOXAL- PHOSPHATE ATTACHMENT SI. | DM00813A 20.30 8.898e-17 231-260 |
| 828 | BL00415 | Synapsins proteins. | BL00415P 2.37 9.814e-09 242-278 |
| 830 | PF00632 | HECT-domain (ubiquitin- | PF00632C 20.66 5.186e-23 1534-1566 |
| | 71.10001.0 | transferase). | PF00632B 18.45 8.393e-22 1480-1508 |
| 831 | DM00215 | PROLINE-RICH PROTEIN 3. | DM00215 19.43 9.695e-09 117-150 |
| 832 | PD01066 | PROTEIN ZINC FINGER ZINC-FINGER METAL- BINDING NU. | PD01066 19.43 4.231e-33 12-51 |
| 834 | BL00120 | Lipases, serine proteins. | BL00120B 11.37 5.846e-09 1319-1334 |
| 836 | DM00813 | AMINOTRANSFERASES CLASS-V PYRIDOXAL- PHOSPHATE ATTACHMENT SI. | DM00813A 20.30 8.898e-17 38-67 |
| 838 | PD00289 | PROTEIN SH3 DOMAIN REPEAT PRESYNA. | PD00289 9.97 8.000e-12 69-83 |
| 840 | BL00053 | Ribosomal protein S8 proteins. | BL00053B 14.56 1.000e-08 900-918 |
| 841 | PR00970 . | ARGININE ADP- RIBOSYLTRANSFERASE SIGNATURE | PR00970D 9.96 3.357e-17 129-146 PR00970A 17.73 8.600e-17 30-52 PR00970E 11.23 6.464e-15 177-193 PR00970B 16.37 2.756e-11 58-77 PR00970C 11.05 9.357e-11 89-104 |
| 842 | BL00250 | TGF-beta family proteins. | BL00250A 21.24 7.120e-25 114-150 BL00250B 27.37 4.774e-18 178-214 |
| 846 | BL00240 | Receptor tyrosine kinase class III proteins. | BL00240B 24.70 7.488e-10 156-180 |
| 848 | BL01095 | Chitinases family 18 proteins. | BL01095B 10.82 5.500e-14 24-36 BL01095C 10.76 7.207e-10 246-258 |
| 849 | BL00027 | 'Homeobox' domain proteins. | BL00027 26.43 2.500e-34 300-343 |
| 850 | PR00318 | ALPHA G-PROTEIN (TRANSDUCIN) SIGNATURE | PR00318A 7.84 7.088e-09 188-204 |
| 851 | PF00969 | Class II histocompatibility antigen, beta domain proteins. | PF00969A 22.07 5.846e-29 12-55 PF00969B 9.97 6.211e-25 56-92 PF00969C 27.72 7.324e-16 95-145 |
| 852 | BL00269 | Mammalian defensins proteins. | BL00269B 19.17 6.824e-21 34-63 BL00269A 8.53 6.108e-18 1-21 |
| 853 | PF00777 | Sialyltransferase family. | PF00777B 29.69 8.767e-10 407-450 |
| 856 | DM00191 | w SPAC8A4.04C RESISTANCE SPAC8A4.05C DAUNORUBICIN. | DM00191D 13.94 9.083e-10 100-139 |

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| SEQ ID NO: | Accession No. | Description | Results* |
|---------------|------------------|--|--|
| 857 | PR00823 | PANCREATIC LIPASE | PR00823A 18.01 3.143c-14 19-37 |
| | 7 11000000 | SIGNATURE | PR00823C 6.88 6.164e-12 56-69 |
| 859 | BL00678 | Trp-Asp (WD) repeat | BL00678 9.67 6.684e-09 243-254 |
| 057 | DEGGGTG | proteins proteins. | 2200010 3101 010010 03 213 25 1 |
| 860 | BL00028 | Zinc finger, C2H2 type, | BL00028 16.07 8.650e-13 425-442 |
| 000 | DEGGGZ | domain proteins. | BL00028 16.07 5.696e-12 508-525 |
| | | domain protonis. | BL00028 16.07 8.826e-12 564-581 |
| | | 1 | BL00028 16.07 7.577e-11 201-218 |
| | 1 | | BL00028 16.07 7.5776-11 536-553 |
| • | | | BL00028 16.07 7.923e-11 341-358 |
| | - | ŀ | BL00028 16.07 8.615e-11 285-302 |
| | | | BL00028 16.07 1.600e-10 592-609 |
| | 1 | | BL00028 16.07 1.000c-10 392-009 BL00028 16.07 2.200c-10 229-246 |
| | | | BL00028 16.07 3.400e-10 257-274 |
| | | l . | BL00028 16.07 5.400e-10 237-274 BL00028 16.07 6.100e-10 313-330 |
| | | | BL00028 16.07 7.000e-10 313-330 |
| | 1 | | BL00028 16.07 7.0006-10 309-380 |
| | | | BL00028 16.07 8.2006-10 397-414 BL00028 16.07 5.114e-09 620-637 |
| 864 | BL01126 | Elongation factor Ts | BL01126A 18.48 5.011e-10 2637-2680 |
| | BLUTTZ6 | proteins. | |
| 865 | BL00353 | HMG1/2 proteins. | BL00353B 11.47 1.330e-13 95-145 |
| | | | BL00353B 11.47 5.692e-11 353-403 |
| 866 | BL00972 | Ubiquitin carboxyl-terminal | BL00972A 11.93 4.600e-18 173-191 |
| | ł | hydrolases family 2 proteins. | BL00972D 22.55 1.947e-13 576-601 |
| | | | BL00972E 20.72 2.038e-11 618-640 |
| 867 | BL00383 | Tyrosine specific protein phosphatases proteins. | BL00383E 10.35 2.756e-12 255-266 |
| 872 | BL00030 | Eukaryotic RNA-binding | BL00030B 7.03 5.737e-09 69-79 |
| | | region RNP-1 proteins. | |
| 873 | BL00303 | S-100/ICaBP type calcium | BL00303B 26.15 4.405e-19 50-87 |
| | | binding protein. | BL00303A 21.77 8.765e-15 3-40 |
| 874 | BL00523 | Sulfatases proteins. | BL00523A 13.36 6,500e-17 41-58 |
| | 1 | | BL00523B 8.64 5.909e-15 89-101 |
| | 1 | | BL00523C 12.64 5.500e-13 140-151 |
| | | | BL00523D 9.89 9.438e-11 293-305 |
| 877 | BL00183 | Ubiquitin-conjugating | BL00183 28.97 1.000c-40 42-90 |
| | | enzymes proteins. | |
| 881 | PR00081 | GLUCOSE/RIBITOL | PR00081B 10.38 6.727e-11 116-128 |
| ••• | 11100001 | DEHYDROGENASE | PR00081A 10.53 3.106e-10 40-58 |
| - | 1 | FAMILY SIGNATURE | 111000011110100011000110100 |
| 882 | BL00183 | Ubiquitin-conjugating | BL00183 28.97 1.391e-39 50-98 |
| | 223103 | enzymes proteins. | |
| 883 | BL00183 | Ubiquitin-conjugating | BL00183 28.97 1.391e-39 50-98 |
| 005 | 2200100 | enzymes proteins. | |
| 888 | BL00027 | 'Homeobox' domain | BL00027 26.43 2.929e-30 232-275 |
| 000 | DE00027 | proteins. | 2555527 251.5 21,276-50 252-275 |

Results include Accession number, sub type, eMatrix p-value and the position of the signature.

TABLE 4

| 445 | SEQ ID NO: | Pfam Model | Description | E-value | Pfam | | | |
|--|------------|-----------------|---|----------|--------|--|--|--|
| 446 | | | | | Score | | | |
| 452 | | | | | | | | |
| 485 WD40 WD domain, G-beta repeat 1.3e-19 78.6 | | | | | | | | |
| 483 | | | WD domain, G-beta repeat | | | | | |
| 1844 | | | | | | | | |
| 485 | | | | | | | | |
| ABC GTP EFTU | | | | | | | | |
| Myosin head | | | Zinc finger, C2H2 type | | | | | |
| ABS | | | Elongation factor Tu family | | | | | |
| 489 | | | Myosin head (motor domain) | | | | | |
| 1992 Pikinase Eukaryotic protein kinase domain 7,9e-85 295; 2 295; 2 295; 3 2 | | | | | | | | |
| SH3 | | | | | | | | |
| A97 Syntaxin | | | | | | | | |
| SCAN SCAN SCAN domain 5.4e-67 236.01 | | | | | | | | |
| P-box | | | | | | | | |
| FHA | | | | | | | | |
| Solution | 499 | F-box | F-box domain | 0.0002 | 28.1 | | | |
| PH | | | FHA domain | | 58.3 | | | |
| CH | | Collagen | | | | | | |
| ATP GI PLM ATP GI GI GI GI GI GI GI G | 507 | PH | PH domain | | 59.5 | | | |
| AT8 | 508 | CH | Calponin homology (CH) domain | | 16.3 | | | |
| Dnal Dnal Dnal domain 6.8e-26 99.5 | 512 | | ATP1G1/PLM/MAT8 family | | 116.3 | | | |
| Section | 516 | DnaJ | DnaJ domain | | 95.1 | | | |
| Section | 519 | DnaJ | | | 99.5 | | | |
| Myosin head | 522 | Glycos_transf_2 | Glycosyl transferases | 1.2e-13 | | | | |
| Acetyltransf | 523 | | Globin | 4.1e-38 | 137.3 | | | |
| Acetyltransf | 526 | myosin head | Myosin head (motor domain) | 0 | 1057.8 | | | |
| MSP domain | 529 | | Acetyltransferase (GNAT) family | 5e-11 | 50.1 | | | |
| Transmembrane receptor (Secretin family) | | | | 1.7e-16 | 68.2 | | | |
| Tropomyosin Tropomyosin 3.1e-173 541.9 | | | 7 transmembrane receptor (Secretin | 1.3e-59 | 211.5 | | | |
| 1.538 LRR | 534 | Tropomyosin | Tropomyosin | 7e-177 | 553.3 | | | |
| 538 LRR Leucine Kich Repeat 2,9e-23 90,7 539 tRNA-synt lb tRNA synthatases class I (W and Y) 7,9e-79 25,3 540 PAS PAS domain 2,8e-05 24,9 541 Ferritin Ferritin 9,9e-116 391,6 549 pro isomerase Cyclophilin type peptidyl-prolyl cis-tr 3,e-33 117,6 549 KH-domain KH domain 0,0004 27,1 551 Glyco transf 8 Glycosyl transferase family 8 0,01 47,7 554 zf-C2H2 Zinc finger, C2H2 type 2,6e-22 87,5 554 zf-C2H2 Zinc finger, C2H2 type 2,6e-22 87,5 555 Arylesterase Aylesterase 2,3e-211 71,5 556 G-patch G-patch domain 2,4e-17 71,1 557 DEAD DEAD/DEAH box helicase 8.7e-67 214.2 559 DSPc Dual specificity phosphatase, catalytic 4.8e-70 246.1 559 DSPc <td< td=""><td></td><td></td><td></td><td>3.1e-173</td><td>541.9</td></td<> | | | | 3.1e-173 | 541.9 | | | |
| 539 dixNA-synt, 1b dfxNA synthetases class I (W and Y) 7,9e-79 275.3 540 PAS PAS PAS domain 2.8e-05 24,9 541 ferritin Ferritin 9,9e-116 391,6 546 pro isomerase Cyclophilin type peptidyl-prolyl cis-tr 3,5e-33 117,6 547 KH-domain KH domain 0,0004 27.1 551 Glyco transf 8 Glycosyl transferase family 8 0,01 47.7 554 zf-C27H2 Zinc finger, C2H2 type 2,6e-22 87.5 555 Arylesterase Arylesterase 2,3e-211 715.6 556 G-patch G-patch domain 2,4e-17 71.1 557 DEAD DEAD/DEAH box helicase 8.7e-67 214.2 558 Methyltransf 4 Putative methyltransferase 0,0095 48.4 559 DSPc Dual specificity phosphatase, catalytic 4.8e-70 246.1 560 zf-C2H2 Zinc finger, C2H2 type 2,6e-19 7.76 | 538 | | | 2.9e-23 | 90.7 | | | |
| PAS | | | | 7.9e-79 | 275.3 | | | |
| 541 ferritin Ferritin 9.9e-116 391.6 546 pro isomerase Cyclophilin type peptidyl-prolyl cis-tr 3.5e-33 11.76 549 KH-domain KH domaln 0.0004 27.1 551 Glyco transf 8 Glycosyl transferase family 8 0.01 47.7 554 zf-C2PL2 Zine finger, C2H2 type 2.6e-22 87.5 555 Arylesterase Arylesterase 2.3e-211 715.6 556 G-patch G-patch domain 2.4e-17 71.5 577 DEAD DEAD/DEAH box helicase 8.7e-67 214.2 588 Methyltransf 4 Putative methyltransferase 0.0095 48.8 559 DSPc Dual specificity phosphatase, catalytic 4.8e-70 246.1 60m r 2.6c-19 7.6 232.4 566 zf-C2H2 Zinc finger, C2H2 type 2.6e-19 7.6 570 RNA_pol_L RNA polymerases L/13 to 16 kDa 0.043 -12.1 571 Armadillo seg <td></td> <td></td> <td></td> <td></td> <td></td> | | | | | | | | |
| 546 pro | | | Ferritin | | | | | |
| 549 KH-domain KH domain 0.0004 27.1 551 Glyeo transf 8 Glyeosyl transferase family 8 0.01 47.7 554 zf-C2H2 Zinc finger, C2H2 type 2.6e-22 87.5 555 Arylesterase Arylesterase 2.3e-211 71.5 556 G-patch G-patch domain 2.4e-17 71.1 557 DEAD DEAD/DEAH box helicase 8.7e-67 214.2 558 Methyltransf 4 Putative methyltransferase 0.0095 48.4 559 DSPc Dual specificity phosphatase, catalytic 4.8e-70 246.1 60m group of the common | | | | | | | | |
| Section | | | | | | | | |
| 26e-22 27.6 | | | | | | | | |
| 555 Arylesterase Arylesterase 2.3e-211 715.6 556 G-patch G-patch domain 2.4e-17 71.1 557 DBAD DBAD/DBAH box helicase 8.7e-67 214.2 558 Methyltransf 4 Putative methyltransferase 0.0095 -48.4 559 DSPc Dual specificity phosphatase, catalytic -0 246.1 563 IPPT IPP transferase 6.7e-66 232.4 566 zFC2H2 Zinc finger, C2H2 bye 2.6e-19 77.6 570 RNA_pol_L RNA polymerases L/ 13 to 16 kDa 0.043 -12.1 subunit subunit 8.6e-33 122.4 571 Armadillo seg Armadillo/tela-catenin-like repeat 8.6e-33 122.4 576 PAP2 PAP3 superfamily 1.2e-19 78.7 577 Defensin propep Defensin propeptide 3e-25 97.3 578 in munoglobulin domain 3.5e-16 57.2 | | | | | | | | |
| 556 G-patch G-patch domain 2.4e-17 71.1 357 DEAD DEAD/DEAH box helicase 8.7e-67 214.2 588 Methyltransf Putative methyltransferase 0.0095 -48.4 559 DSPc Dual specificity phosphatase, catalytic dom 4.8e-70 246.1 561 DFPT IPP Transferase 6.7e-66 232.4 566 zFC2H2 Zinc finger, C2H2 type 2.6e-19 77.6 570 RNA_pol_L RNA polymerases L/13 to 16 kDa submit 0.043 -12.1 571 Armadillo seg Armadillo/beta-catenin-like repeat 8.6e-33 122.4 574 WD40 WD domain, G-beta repeat 1.1e-65 231.6 576 PAP2 PAP2 superfamily 1.2e-19 78.7 577 Defensin, propep Defensin propeptide 3e-25 97.3 578 ig Immunoglobulin domain 3.5e-16 57.2 | | | | | | | | |
| 557 DEAD DEAD/DEAH box helicase 8.7e-67 214.2 558 Methyltransf 4 Putative methyltransferase 0.0095 -48.4 559 DSPc Dual specificity phosphatase, catalytic dom 48e-70 246.1 563 IPPT IPP ransferase 6.7e-66 232.4 566 zf-C2H2 Zinc finger, C2H2 type 2.6e-19 77.6 570 RNA pol_L RNA polymerases L / 13 to 16 kDa subunit 0.043 -12.1 571 Armadillo seg Armadillo/tela-catenin-like repeat 8.6e-33 122.4 574 WD40 WD domain, 6-bear repeat 1.1e-65 231.6 576 PAP2 PAP2 superfamily 1.2e-19 78.7 577 Defensin_propep Defensin_propeptide 3e-25 97.3 578 ig Immunoglobulin domain 3.5e-16 57.2 | | | | | | | | |
| 558 Methyltransf 4 Putative methyltransferase 0.0095 48.4 559 DSPc Dual specificity phosphatase, catalytic dom 246.1 246.1 563 IPPT IPP transferase 6.7e-66 232.4 566 zf-C2H2 Zinc finger, C2H2 type 2.6e-19 77.6 570 RNA_pol_L RNA polymerases L/13 to 16 kDa subunit 0.043 -12.1 571 Armadillo seg Armadillo/seta-catenin-like repeat 8.6e-33 122.4 574 WD40 WD domain, G-beta repeat 1.1e-65 231.6 576 PAP2 superfamily 1.2e-19 78.7 577 Defensin_propep Defensin_propeptide 3e-25 97.3 578 ig Immunoglobulin domain 3.5e-16 57.2 | | | | | | | | |
| DSPc Dual specificity phosphatase, catalytic dom 246.1 | | | | | | | | |
| 563 IPPT IPP transferase 6.7e-66 23.2.4 566 zFCZHZ Zinc finger, CZH2 type 2.6e-19 77.6 570 RNA_pol_L RNA polymerases L/13 to 16 kDa 0.043 -12.1 571 Armadillo seg Armadillo/beta-catenin-like repeat 8.6e-33 122.4 574 WD40 WD domain, G-beta repeat 1.1e-65 231.6 576 PAP2 PAP2 superfamily 1.2e-19 78.7 577 Defensin_propep Defeasin_propeptide 3e-25 97.3 578 ig Immunoglobulia domain 3.5e-16 57.2 | | | Dual specificity phosphatase, catalytic | | | | | |
| 566 zf-C2H2 Zinc finger, C2H2 type 2.6e-19 77.6 570 RNA_pol_L RNA polymerases L/13 to 16 kDa subunit 0.043 -12.1 571 Armadillo seg Armadillo/tela-catenin-like repeat 8.6e-33 122.4 574 WD40 WD domain, 6-bear repeat 1.1e-65 231.6 576 PAF2 PAP2 superfamily 1.2e-19 78.7 577 Defensin_propep Defensin_propeptide 3e-25 97.3 578 ig Immunoglobulin domain 3.5e-16 57.2 | 563 | IPPT | IPP transferase | 6.7e-66 | 232.4 | | | |
| 570 RNA_pol_L subunit RNA_pol_verses L/13 to 16 kDa subunit 0.043 -12.1 571 Armadillo seg Armadillo/beta-catenin-like repeat 8.6e-33 122.4 574 WD40 WD domain, G-beta repeat 1.1e-65 231.6 576 PAP2 PPAP2 superfamily 1.2e-19 78.7 577 Defensin_propep Defensin_propeptide 3e-25 97.3 578 ig Immunoglobulin domain 3.5e-16 57.2 | | | | | | | | |
| 571 Armadillo seg Armadillo/beta-catenin-like repeat 8.6e-33 122.4 574 WD40 WD domain, G-beta repeat 1.1e-65 23.1e 576 PAP2 SPAP2 superfamily 1.2e-19 78.7 577 Defensin propep Defensin propeptide 3e-25 97.3 578 jig Immunoglobulin domain 3.5e-16 57.2 | | | RNA polymerases L / 13 to 16 kDa | | | | | |
| 574 WD40 WD domain, G-beta repeat 1.1e-65 231.6 576 PAP2 PAP2 superfamily 1.2e-19 78.7 577 Defensin propep Defensin propeptide 3e-25 97.3 578 ig Immunoglobulin domain 3.5e-16 57.2 | 571 | Armadillo seg | | 8.6e-33 | 122.4 | | | |
| 576 PAP2 PAP2 superfamily 1.2e-19 78.7 577 Defensin propep Defensin propeptide 3e-25 97.3 578 ig Immunoglobulin domain 3.5e-16 57.2 | | | | | | | | |
| 577 Defensin propep Defensin propeptide 3e-25 97.3 578 ig Immunoglobulin domain 3.5e-16 57.2 | | | | | | | | |
| 578 ig Immunoglobulin domain 3.5e-16 57.2 | | | | | | | | |
| | | | | | | | | |
| 1 NO PIR PIA kingse Phoenhatidylinositol 3- and 4-kingse 6 5e-93 1 322 1 | 580 | PI3 PI4 kinase | Phosphatidylinositol 3- and 4-kinase | 6.5e-93 | 322.1 | | | |

| SEQ ID NO: | Pfam Model | Description | E-value | Pfam Score |
|------------|---------------------|--|----------|---------------|
| 585 | GBP | Guanylate-binding protein, N-terminal domain | 4.3e-165 | 548.2 |
| 586 | PGM_PMM_I | Phosphoglucomutase/phosphomannom utase, alp | 7.6e-06 | 4.4 |
| 587 | zf-C3HC4 | Zinc finger, C3HC4 type (RING finger) | 1.3e-11 | 41.9 |
| 588 | MMR HSR1 | GTPase of unknown function | 5.9e-48 | 172.7 |
| 590 | zf-DHHC | DHHC zinc finger domain | 1.8e-36 | 134.6 |
| 591 | Ribosomal_S3_C | Ribosomal protein S3, C-terminal domai | 1.3e-07 | 28.0 |
| 592 | LIM | LIM domain | 4.4e-27 | 103.4 |
| 594 | pkinase | Protein kinase domain | 3.7e-77 | 269.7 |
| 596 | PX | PX domain | 2.2e-17 | 71.2 |
| 599 | Cadherin C term | Cadherin cytoplasmic region | 3.3e-88 | 306.5 |
| 600 | FHA | FHA domain | 3.4e-20 | 80.5 |
| 601 | Acetyltransf | Acetyltransferase (GNAT) family | 3.2e-17 | 70.6 |
| 604 | NAP_family | Nucleosome assembly protein (NAP) | 5.5e-12 | 46.4 |
| 605 | RhoGAP | RhoGAP domain | 1e-28 | 108.9 |
| 606 | Armadillo seg | Armadillo/beta-catenin-like repeat | 0.00022 | 28.0 |
| 607 | pkinase | Protein kinase domain | 5.9e-77 | 269.1 |
| 608 | zf-C2H2 | Zinc finger, C2H2 type | 5.4e-110 | 378.8 |
| 609 | ras | Ras family | 1.2e-16 | |
| 610 | | | | 52.8 |
| 612 | ank | Ank repeat | 1.6e-08 | 41.8 |
| 613 | pkinase WD40 | Protein kinase domain | 1.6e-69 | 244.3 |
| | | WD domain, G-beta repeat | 4.7e-55 | 196.3 |
| 614 | UBA | UBA/TS-N domain | 3.6e-12 | 53.9 |
| 615 | Zip | ZIP Zinc transporter | 8.1e-59 | 208.8 |
| 618 | sushi | Sushi domain (SCR repeat) | 1.3e-58 | 208.2 |
| 619 | K_tetra | K+ channel tetramerisation domain | 1.3e-19 | 78.6 |
| 621 | CAP_GLY | CAP-Gly domain | 1.9e-48 | 174.3 |
| 622 | TCTP | Translationally controlled tumor protein | 5.2e-109 | 375.5 |
| 628 | UQ_con | Ubiquitin-conjugating enzyme | 0.0046 | -43.3 |
| 629 | DPPIV_N_term | Dipeptidyl peptidase IV (DPP IV) N- termi | 5.1e-07 | -82.1 |
| 630 | DPPIV_N_term | Dipeptidyl peptidase IV (DPP IV) N- termi | 5.5e-07 | -83.2 |
| 631 | efhand | EF hand | 2.3e-14 | 61.1 |
| 632 | Pribosyltran | Phosphoribosyl transferase domain | 4.3e-37 | 136.7 |
| 635 | ank | Ank repeat | 1.8e-25 | 98.0 |
| 636 | MHCK_EF2_kinas e | MHCK/EF2 kinase domain family | 1.2e-12 | 5.6 |
| 637 | DUF221 | Domain of unknown function DUF221 | 1.2e-89 | 311.2 |
| 639 | bromodomain | Bromodomain | 2.2e-29 | 106.0 |
| 641 | ubiquitin | Ubiquitin family | 2.2e-21 | 81.9 |
| 644 | RIO1 | RIO1/ZK632.3/MJ0444 family | 1.1e-07 | -14.9 |
| 646 | NDK | Nucleoside diphosphate kinase | 1.1e-52 | 188.4 |
| 649 | zf-C3HC4 | Zinc finger, C3HC4 type (RING finger) | 9.4e-12 | 42.4 |
| 651 | ABC tran | ABC transporter | 7.9e-84 | 291.9 |
| 654 | CUB | CUB domain | 3e-30 | 113.9 |
| 655 | MHCK_EF2_kinas | MHCK/EF2 kinase domain family | 2.6e-09 | -35.3 |
| | е | | | 1 |
| 659 | zf-C3HC4 | Zinc finger, C3HC4 type (RING finger) | 1.3e-11 | 41.9 |
| 661 | UvrD-helicase | UvrD/REP helicase | 0.078 | 9.7 |
| 663 | TFIIS | Transcription factor S-II (TFIIS) | 2e-22 | 87.9 |
| 664 | dsrm | Double-stranded RNA binding motif | 4.3e-42 | 153.3 |
| 665 | rrm | RNA recognition motif. | 0.002 | 24.8 |
| 669 | OTU | OTU-like cysteine protease | 1e-19 | 78.9 |
| 671 | TFIIS | Transcription factor S-II (TFIIS) | 2e-22 | 87.9 |
| 672 | zf-C3HC4 | Zinc finger, C3HC4 type (RING finger) | 1.5e-05 | 22.3 |
| 673 | AMP-binding | AMP-binding enzyme | 1.6e-86 | 300.9 |
| | | | | |

| SEQ ID NO: | Pfam Model | Description | E-value | Pfam Score |
|------------|----------------|---|---------|---------------|
| 679 | MSP_domain | MSP (Major sperm protein) domain | 5.4e-18 | 73.2 |
| 680 | MSP_domain | MSP (Major sperm protein) domain | 5.5e-11 | 49.9 |
| 683 | RNase PH | 3' exoribonuclease family | 3e-42 | 153.8 |
| 684 | lactamase_B | Metallo-beta-lactamase superfamily | 0.088 | -15.6 |
| 686 | tRNA anti | OB-fold nucleic acid binding domain | 0.031 | 20.9 |
| 690 | NHL | NHL repeat | 8.2e-18 | 72.6 |
| 691 | zf-C3HC4 | Zinc finger, C3HC4 type (RING finger) | 6.1e-09 | 33.2 |
| 693 | WD40 | WD domain, G-beta repeat | 0.025 | 21.2 |
| 694 | WD40 | WD domain, G-beta repeat | 1.1e-23 | 92.1 |
| 696 | Choline_kinase | Choline/ethanolamine kinase | 1.6e-51 | 184.6 |
| 697 | zf-C2H2 | Zinc finger, C2H2 type | 3.4e-74 | 259.9 |
| 698 | cadherin | Cadherin domain | 2.2e-05 | 31.3 |
| 701 | PRK | Phosphoribulokinase / Uridine kinase family | 1.1e-79 | 278.1 |
| 702 | DnaJ | DnaJ domain | 5e-26 | 99.9 |
| 888 | PAX | 'Paired box' domain | 1.1e-87 | 304.7 |

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|----------------|---|---|---|---|---|--|--|--|--|--|---------------------------|
| PDB annotation | OXIDOREDUCTASE PDZ DOMAIN, NNOS, NITRIC OXIDE SYNTHASE | PEPTIDE RECOGNITION PEPTIDE RECOGNITION, PROTEIN LOCALIZATION | CYTOKINE LCF: CYTOKINE, LYMPHOCYTE CHEMOATTRACTANT FACTOR, PDZ DOMAIN | KINASE HCASK, GLGF REPEAT, DHR; PDZ DOMAIN, NEUREXIN, SYNDECAN, RECEPTOR CLUSTERING, KINASE | OXIDOREDUCTASE BETA-FINGER | MEMBRANE PROTEIN/OXIDORED/JCTASE BETA- FINGER, HETERODIMER | HYDROLASE PDZ DOMAIN, HUMAN PHOSPHATASB, HPTP1E, PTP-BAS, SPECIFICITY 2 OF BINDING | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) |
| Coumpound | NEURONAL NITRIC OXIDE SYNTHASE; CHAIN: A; HEPTAPEPTIDE; CHAIN: B; | PSD-95; CHAIN: A; CRIPT; CHAIN: B; | INTERLEUKIN 16; CHAIN: NULL; | HCASK/LIN-2 PROTEIN; CHAIN: A, B; | NEURONAL NITRIC OXIDE SYNTHASE (RESIDUES 1- 130); CHAIN: A: | ALPHA-I SYNTROPHIN (RESIDUES 77-171); CHAIN: A; NEURONAL NITRIC OXIDE SYNTHASE (RESIDUES 1-130); CHAIN: B: | TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1); CHAIN: A; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUFLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE: CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | QGSR ZINC FINGER PEPTIDE: CHAIN: A: DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | QGSR ZINC FINGER |
| SeqFold | | | | | | | | | | 80.51 | |
| PMF | 0.99 | 9.65 | 0.48 | 8.0 | _ | 0.81 | 0.74 | _ | 0.11 | | _ |
| Verify | 0.39 | -0.32 | 0.58 | 0.26 | 0.7 | 0.2 | 0.64 | 0.24 | -0.03 | | 91.0 |
| PSI- BLAST | 1.30E-07 | 0.00014 | 1.30E-05 | 1.10E-11 | 7.00E-11 | 5.60E-10 | 2.80E-05 | 1.70E-30 | 1.70E-23 | 4.20E-29 | 4.20E-29 |
| End | 401 | 401 | 414 | 404 | 410 | 396 | 414 | 189 | 248 | 278 | 277 |
| Start | 324 | 355 | 329 | 329 | 325 | 324 | 324 | 109 | 137 | 194 | 195 |
| Chain | ¥ | ¥ | | 4 | ٧ | ∢ | 4 | V | ¥ | ٧ | < |
| EDB ED | 1589 | 1be9 | 1116 | Ikwa | lqau | lqav | 3pdz | lalh | lalh | lath | lalh |
| SEQ E | 44 5 | 445 | 445 | 445 | \$# | 445 | 445 | 446 | 446 | 446 | 446 |

| PDB annotation | FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA FINTERACTION, ROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FROGER/DNA) |
|------------------|---|--|--|---|---|---|---|--|--|--|
| Coumpound | OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B, C: | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSK ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B, C: | QGSR ZINC FINGER PEPTIDE: CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; |
| SeqFold score | | | | | | | | | | |
| PMF | | 1 | _ | 0.99 | _ | 0.05 | 0.21 | - | 56:0 | 0.98 |
| Verify | | -0.05 | -0.09 | -0.18 | -0.24 | 0.1 | -0.35 | 0.35 | 0.38 | 0.11 |
| PSI- BLAST | | 6.80E-28 | 8.50E-28 | 1.50E-28 | 1.20E-30 | 5.10E-20 | 4.20E-25 | 1.20E-49 | 1.70E-38 | 1.00E-44 |
| End AA | | 276 | 303 | 331 | 359 | 133 | 189 | 189 | 220 | 276 |
| Start AA | | 202 | 224 | 252 | 280 | 83 | 18 | 108 | 136 | 291 |
| Chain ID | | ∢ | ¥ | | ٧ | ¥ | V | ပ | ပ | U |
| 808 CD | | lalh | lalh | lalh | lalh | laIh | lalh | lme y | J me | Ime y |
| S e S | | 446 | 446 | 446 | 446 | 446 | 446 | 446 | 446 | 446 |

| | | | | | , | | | | |
|------------------|--|--|--|--|--|--|--|---|------------------------|
| PDB annotation | COMPLEX (ZINC FINGERJDNA) ZINC FINGER, PROTEIN-DDNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA FINERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERIDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERIDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (TRANSCRIPTION |
| Coumpound | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN: CHAIN: C, F, G; | DNA, CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN: CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | TRANSCRIPTION FACTOR |
| SeqFold score | | | 97.55 | | | | | | 62.34 |
| PMF | - | -0.13 | | _ | 0.75 | - | 0.36 | 0.19 | |
| Verify | 0.15 | 0.08 | | 0.11 | 0.19 | 0.53 | -0.13 | 0.39 | |
| PSI- BLAST | 1.70E-47 | 5.10E-21 | 1.00E-48 | 1.00E-48 | 5.10E-37 | 1.00E-48 | 4.20E-27 | 5.10E-12 | 1.20E-20 |
| End | 303 | 105 | 360 | 360 | 133 | 191 | 190 | 105 | 192 |
| Start AA | 223 | 27 | 278 | 279 | | 80 | 83 | | 108 |
| Chain El El | v | ပ | ပ | ပ | U | U | ပ | 5 | A |
| 80 a. | J me | y y | Ime y | Jme y | y y | y y | Jme y | y me | 9 |
| SEQ NO: DE | 446 | 446 | 446 | 446 | 446 | 446 | 446 | 446 | 446 |

| PDB annotation | RECULATION/DNA) TFULA; 5S GENE; NNAC, FILIAL, ROTGEN, DNA, TRANSCRIPTION FACTOR, 5S RNA 2 GENE, DNA, BINDING PROTEIN, ZINC FINGER, COMPLEX.) (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATIONDNA) TIFILA; SS GENE; NMR, TEILA, PROTEN, DNA, TRANSCRIPTION FACTOR, SS TNA 2 GENE, DNA BINDING PROTEIN, ZINC FINGER, COMPLEX; | COMPLEX (TRANSCRIPTION REGULATIONIDNA) TEIIA; SS GENE; NMR, TEIIA, PROTEN, DNA; TRANSCRIPTION FACTOR, SS RNA 2 GENE, DNA BINDING PROTEIN, ZINC FINGER, COMPLEX; | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION MITTATION, ZNC PRIGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONINA) COMPLEX (TRANSCRIPTION REGULATIONINA), RNA REGULATIONINA), RNA POLYMERASE III, 2 TRANSCRIPTION MITTATION, ZNC ENGRR PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONINA) COMPLEX (TRANSCRIPTION REGULATIONINA), RNA REGULATIONINA), RNA POLYMERASE III, 2 TRANSCRIPTION NITIATION, ZNC FINGRE PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION |
|------------------|---|---|--|---|---|--|--|
| Coumpound | IIIA; CHAIN: A; SS RNA GENE; CHAIN: E, F; | TRANSCRIPTION FACTOR IIIA, CHAIN: A, 58 RNA GENE, CHAIN: E, F, | TRANSCRIPTION PACTOR IIIA; CHAIN: A, 58 RNA GENE, CHAIN: E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL, RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL, RNA GENE; CHAIN: B, C, E, F, | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; |
| SeqFold score | | | | 124.38 | | | |
| PMF | | 0.53 | 0.05 | | 0.94 | 0.99 | 0.86 |
| Verify score | | 0.22 | -0.07 | | 0.37 | -0.14 | 0.11 |
| PSI- BLAST | | 1,20E-20 | 1.00E-14 | 1.70E-36 | 1.70E-36 | 1.40E-35 | 3.40E-30 |
| End AA | | 681 | 129 | 281 | 257 | 347 | 189 |
| Start AA | | 601 | 09 | 801 | 601 | 204 | 09 |
| Chain 10 | | ¥ | ∢ | Ą | ¥ | ¥ | Ą |
| EDB ED | | 91 | G 11 | 1116 | 1116 | 1146 | 146 |
| Se Se Se | | 446 | 446 | 446 | 446 | 446 | 446 |

| | | | | | | • | • |
|-----------------|---|--|--|---|---|---|--|
| PDB annotation | REGULATIONDIA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION NITTATION, ZNC, FINGER PROTEIN | COMPLEX (TRANSCRIPTION REQUILATIONDNA YING-YANG I; TRANSCRIPTION INITATION, INITATIOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION, COMPLEX TRANSCRIPTION REGULATIONDNA | COMPLEX (TRANSCRIPTION REGULATIONDNA, YNG-YANG I; TRANSCRIPTON INITIATION, INITIATOR ELEMENT, YYI, ZMC2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATIONDNA, YNG-YANG I; TRANSCRIPTON INITIATION, INITIATIOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION, 3 COMPLEX TRANSCRIPTON REGULATIONDNA | COMPLEX (TRANSCRIPTION REGIL,ATIONDNA) YING-YANG I; TRANSCRIPTION INTATION, INITATIOR RELABENT, YYI, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION, 3 COMPLEX TRANSCRIPTION REGILATIONDNA | COMPLEX (TRANSCRIPTION REGULATIONIDNA) YING-YANG 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 |
| Coumpound | | TFILIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INTIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DINA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED YIRUS PS INITIATOR ELEMENT DINA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INTIATOR ELEMENT DINA; CHAIN: A, B; | YYI; CHAIN: C; ADENO. ASSOCIATED YIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B: |
| SeqFold | | | | | | | |
| PMF | | 0.87 | 0.92 | 96.0 | 0.72 | - | 0.98 |
| Verify score | | -0.04 | -0.12 | 10.0 | 0.01 | 60:0 | -0.01 |
| PSI- BLAST | | 8.50E-32 | 2.80E-32 | 1.70E-28 | 1.50E-30 | 2.80E-35 | 9.80E-36 |
| End | | 229 | 248 | 220 | 276 | 276 | 331 |
| Start | | 18 | 106 | 116 | 144 | 169 | 861 |
| Chain | | ď | U | ပ | ပ | U | O |
| EDB EDB | |)H2 | 1ubd | Inpq | Tubd | Jubd . | lubd |
| Š a Š | | 446 | 446 | 446 | 446 | 446 | 446 |

| PDB annotation | FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, INITIATOR FLEMENT, YYL, ZINC.2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | INCLUSION INTERNATION, | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | KEGULAHUN/DNA) YING-YANG I; | DIMANSCRIPTION INITIATION, | ENGER PROTEIN DNA-PROTEIN | RECOGNITION 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YYI, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGILL ATTOM/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG I; TRANSCRIPTION INITIATION. |
|-----------------|---|---|--|-----------------------------|---|------------------------|------------------------------|------------------------|-----------------------------|------------------------|--------------------------------|------------------------|-----------------------------|----------------------------|---------------------------|-----------------------|--------------------------------|------------------------|------------------------------|---------------------------|--------------------------------|-----------------------------|---|------------------------|------------------------------|---------------------------|--------------------------------|-----------------------------|------------------------|--------------------------------|------------------------|---|
| Coumpound | | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | (a (v : wa) | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | CHAIN: A. B. | 1 | | | YYI; CHAIN: C; ADENO- | ASSOCIATED VIKUS PS | CHAIL A P. | CIPAIN: A, B, | | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | YY1; CHAIN: C. ADENO- | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; |
| SeqFold | | | | | | | | | | | | 10:501 | | | | | | | | | | | | | | | | | | | | |
| PMF score | | 0.93 | | | | - | | | | | | | | | | | | _ | | | | | | 0.11 | | | | | | | _ | |
| Verify score | | 80.0 | | | | -0.08 | | | | | | | | | | | | 10.0 | | | | | | 0.24 | | | | | | | 0.37 | |
| PSI- BLAST | | 5.10E-32 | | | | 2.80E-31 | | | | | | 9.80E-36 | | | | | | 3.40E-34 | | | | | | 5.10E-23 | | | | | | | 5.10E-30 | |
| End AA | | 303 | | | | 329 | | | | | | 360 | | | | | | 359 | | | | | | 133 | | | | | | | 19 | |
| Start | | 205 | | | | 221 | | | | | | 253 | | | | | | 256 | | | | | | 27 | | | | | | | 8 | |
| Chain | | S | | | | O | | | | | | ပ | | | | | | O | | | | | | O | | | | | | | ပ | |
| ED ED | | Inpd | | | | 1ubd | | | | | | Inpq | | _ | | | | Inpq | | | | | | lubd | | | | | | | lubd | |
| Se Se | | 446 | | | | 446 | | | | | | 446 | _ | | | | | 4 | | | | | | 446 | | | | | | | 446 | |

| PDB annotation | INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATIONDNAN YING-YANG 1; TRANSCRIPTION INTIATION; INTIATION ELEMBET, YYI, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION; COMPLEX | (IKANSCRIPTION REGULATION IN TRANSCRIPTION REGULATION TRANSCRIPTION REGULATION, ADRIL ZINC FINGER, NMR | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZNC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- |
|-----------------|---|--|--|--|--|--|--|--|---|--|
| Coumpound | CHAIN: A, B; | YYI; CHAIN: C; ADENO. ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | ADRI; CHAIN: NULL; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLI1; CHAIN: A: DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; |
| SeqFold | | | | | | | 99.39 | | | |
| PMF | | 66.0 | -0.19 | 0.21 | 0.11 | _ | | _ | _ | 0.4 |
| Verify score | | 0.11 | 0.04 | 0.05 | 90.04 | 0.11 | | 0.46 | 0.27 | 0.48 |
| PSI- BLAST | 0 | 1.40E-32 | 1.70E-09 | 2.80E-42 | 5.10E-29 | 1.10E-41 | 2.80E-42 | 3.40E-30 | 3.40E-32 | 3.40E-27 |
| End . | | 681 | 107 | 331 | 275 | 359 | 333 | 330 | 358 | 160 |
| Start | | 28 | 23 | 601 | 116 | 165 | . 195 | 207 | 231 | 32 |
| Chain D | | ပ | | ·4 | ∀ | ∢ | ∢ | ∢ | ∢ | 4 |
| EQ. | | Jubd | 2adr | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli |
| SE B SE | | 446 | 446 | 446 | 446 | 446 | 446 | 446 | 446 | 446 |

| | _ | | | | | | | | | | | | | _ | | | | | | | | | | | | | |
|-----------------|----------------------|--|--|--|----------------------------|-------------------------------|--|----------------------------|---------------------------|------------------------------|--------------------|------------------------|----------------------------|----------------------------|--|-------------------------|----------------------------|---------------------------|-----------------------------|--------------------|------------------------|----------------------------|---------------------------|--|-----------------------|--|---|
| PDB annotation | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINIDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINIDNA) | COMPLEX (DNA-BINDING PROTEINIDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINIDNA) | CYTOSKELETON ELASTICITY, MEMBRANE SKELETON, SPECTRIN, COILED-COIL, 2 CYTOSKELETON, | CALMODULIN-BINDING, ACTIN- | CALCIUM-BINDING, DUPLICATION, | REPEAT, 4 SH3 DOMAIN | DEBEATS OF SPECTRIN AT BLA | HELICAL LINKER REGION, 22 | TANDEM 3-HELIX COILED-COILS, | STRUCTURAL PROTEIN | STRUCTURAL PROTEIN TWO | REPEATS OF SPECTRIN, ALPHA | HELICAL LINKER REGION, 2 2 | TANDEM 3-HELIX COILED-COILS, STRIICTHRAL PROTEIN | STRIICTIRAL PROTEIN TWO | REPEATS OF SPECTRIN, ALPHA | HELICAL LINKER REGION, 22 | TANDEM 3-HELIX COILED-COILS | STRUCTURAL PROTEIN | STRUCTURAL PROTEIN TWO | REPEATS OF SPECTRIN, ALPHA | HELICAL LINKER REGION, 22 | TANDEM 3-HELIX COILED-COILS, crelicated to the control of the cont | MENDE AND THE PROTEIN | MEMBANANE FRO I ELIN FOUR HELLA BUNDLE, ALPHA HELIX | CONTRACTILE PROTEIN TRIPLE- HELIX COILED COIL, CONTRACTILE |
| Coumpound | | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ALPHA SPECTRIN; CHAIN: NULL; | • | | A CONTRACTOR OF THE CONTRACTOR | ALPHA SPECIKIN; CHAIN: | γ, Β, C, | | | ALPHA SPECTRIN; CHAIN: | A, B, C; | | | AI PHA SPECTRIN: CHAIN: | A. B. C. | | | | ALPHA SPECTRIN; CHAIN: | A, B, C; | | | SEOI BEOTER! CITAR! 4 | SOUT FROIDIN, CHAIN: A; | HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: |
| SeqFold | | | | | | | | | | | | | | | | 573 | | | | | | | | | | | 64.46 |
| PMF score | | 0.93 | 1 | 0.09 | | | | 57.0 | | | | 0.03 | | | | | | | | | 0.33 | | | | 0.00 | 67.0 | |
| Verify score | | -0.1 | 0.31 | 0.28 | | | 100 | 17:0- | | | | -0.17 | | | | | | | | | -0.07 | | | | 0.33 | 30.0 | |
| PSI- BLAST | | 2.80E-45 | 8.50E-31 | 6.80E-16 | | | 1 000 | 1.005-1/ | | | | 5.60E-05 | | | | 1.70E-23 | ! | | | | 1.70E-23 | | | | 0.00028 | 0.00020 | 1.70E-19 |
| End AA | | 278 | 247 | 139 | | | 9, | 741 | | | | 201 | | | | 262 | | | | | 259 | | | | 121 | 131 | 267 |
| Start | | 83 | 88 | 39 | | | , | 7 | | | | ۳. | | | | 37 | | | | | 38 | | | | 2 - | 21 | 23 |
| Chain | | ν | A | | | | | | | | | ∢ | | | | 4 | _ | | | | Ą | | | | | | ٧ |
| PDB ID | | 2gli | 2gli | laj3 | | | | IIcon | | | 1 | Icun | | | | Icun | | | | | Icun | | | | Ę. | , , | lqu |
| S e S | | 446 | 446 | 447 | | | 447 | Ì | | | | 447 | | _ | | 447 | | | | | 447 | | | | 447 | | 447 |

| | | | | | | | _ | | | _ | | _ | | _ | | | _ | _ | | _ | | | | _ |
|-----------------|---------|--|--|----------------------------|---|---|----------------------------------|---|---|-------------------------------|---------------------------------|-------------------------------|--|-------------------------------|---------------------------------|-------------------------------|----------------|---|---|---|--|---------------------|---|----------------------------|
| PDB annotation | PROTEIN | CONTRACTILE PROTEIN TRIPLE- HELIX COILED COIL, CONTRACTILE PROTEIN | CONTRACTILE PROTEIN TRIPLE. HELIX COILED COIL, CONTRACTILE PROTEIN | CHAPERONE HOP, TPR-DOMAIN, | PEPTIDE-COMPLEX, HELICAL REPEAT, HSP90, 2 PROTEIN BINDING | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELICAL BEDEAT HORD ADDITION OF THE ACT HORDS | NECEMI, HOLYO, & FROIEIN BINDING | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELICAL | REPEAT, HSC70, 2 HSP70, PROTEIN RINDING | SIGNALING PROTEIN PEROXISMORE | RECEPTOR 1, PTS1-BP, PEROXIN-5, | PTS1 PROTEIN-PEPTIDE COMPLEX, | IEIKAIKIOOFEFIIDE KEFEAI, IFK, Z HELICAL REPEAT | SIGNALING PROTEIN PEROXISMORE | RECEPTOR 1, PTS1-BP, PEROXIN-5, | PISI PROTEIN-PEPTIDE COMPLEX, | HELICAL REPEAT | | TRANSCRIPTION INHIBITOR BETA- PROPELLER | | METHYLTRANSFERASE METHYLTRANSFERASE, CUEMOTA VIS BECEBEDD | METHYLATION | METHYLTRANSFERASE GNMT, S. ADENOSYL-L-METHIONINE: | OCICINE METHICIPANSI ENASE |
| Coumpound | A; | HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A; | HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A; | TPR2A-DOMAIN OF HOP: | CHAIN: A; HSP90-PEPTIDE MEEVD; CHAIN: B; | TPR2A-DOMAIN OF HOP; CHAIN: A; HSP90-PEPTIDE | MEEV D, CHAIN. B, | TPR1-DOMAIN OF HOP; CHAIN: A, B; HSC70- | PEPTIDE; CHAIN: C, D; | PEROXISOMAL TARGETING | SIGNAL I RECEPTOR; | CHAIN: A, B; PTSI- | CHAIN: C, D; | PEROXISOMAL TARGETING | SIGNAL I RECEPTOR; | CONTAINS BESTEDS: | CHAIN: C, D; | | TRANSCRIPTIONAL REPRESSOR TUPI; CHAIN: A, B, C; | | CHEMOTAXIS RECEPTOR METHYL TRANSFERASE CUEB. CUAIN. MILLI. | CHER, CHAIN: INDEE, | GLYCINE N. METHYLTRANSFERASE; | CIDIN, D, B, |
| SeqFold | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.16 | 0.11 | 0.27 | | 0 | | 63 | | 91.0 | | | | 0.49 | | | | | 0.19 | | 0.29 | | 0.21 | |
| Verify score | | -0.31 | -0.19 | -0.26 | | -0.49 | | 0.41 | | -0.37 | | | | 0.12 | | | | | 0.01 | | -0.22 | | -0.32 | |
| PSI- BLAST | | 0.0012 | 1.70E-19 | 5.10E-05 | | 0.0014 | | 1.20E-08 | | 0.0084 | | | | 4.20E-07 | | | | | 5.10E-38 | | 0.0098 | | 2.80E-06 | |
| End AA | | 322 | 265 | 190 | | 220 | 1 | 186 | | 278 | | | | 280 | | | | | 213 | | 146 | | 148 | |
| Start AA | | 256 | 27 | 110 | | 128 | I | <u> </u> | | 128 | | | | 289 | | | | | 4 | | 2 | | 8 | |
| Chain ID | | Α. | V. | ٧ | | < | 1 | ⋖ | | ٧ | | | | _ V | | | | | 4 | | | | - | |
| E G | | Iquu | nnbl | lelr | | lel. | 1 | lelw | | 멸 | | | | 1fch | _ | | | 1 | Ē | | laf7 | | lxva | \prod |
| SEQ No. ii | | 447 | 447 | 450 | | 450 | 1 | 450 | | 420 | | | | 450 | _ | | | | 452 | | 458 | | 428 | |

| PDB annotation | LIM DOMAIN CONTAINING PROTEINS LIM DOMAIN CONTAINING PROTEINS, METAL-BINDING PROTEIN, ZINC 2 FINGER | CLATHRIN CLATHRIN, TRISKELION, COATED VESICLES, ENDOCYTOSIS, SELF-2 ASSEMBLY, ALPHA-ALPHA SUPERHELIX | SIGNALING PROTEIN LIM DOMAIN CONTAINING PROTEINS, METAL- BINDING PROTEIN | TOXIN BINDING PROTEIN TWO DOMAINS: BETA PROPELLER AND ALPHABETA FOLD | TOXIN BINDING PROTEIN TWO DOMAINS: BETA PROPELLER AND ALPHABETA FOLD | TRANSCRIPTION INHIBITOR BETA- PROPELLER | COMPLEX (GTD- BRUNIOGTTANSDUCER, BETA1, TRANSDUCIN BETA SUBUNT: GAMMA, TRANSDUCIN GAMMA SUBUNT: COMPLEX (GTP- BRDDING/TRANSDUCER), G PROTEIN, HETROTRIAMER 2 SIGNAL. |
|-----------------|---|---|--|--|--|---|---|---|---|---|--|
| Coumpound | QCRP2 (LIMI); CHAIN: NULL; | CLATHRIN HEAVY CHAIN; CHAIN: A; | CYSTEINE AND GLYCINE- RICH PROTEIN CRP2; CHAIN: A; | TOLB PROTEIN; CHAIN: A; | TOLB PROTEIN; CHAIN: A; | TRANSCRIPTIONAL REPRESSOR TUP1; CHAIN: A, B, C; | TRANSCRIPTIONAL REPRESSOR TUPI; CHAIN: A, B, C; | GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT- BETA; CHAIN: B; GT- GAMMA; CHAIN: G; |
| SeqFold | | | | | | | | | | | 101.01 |
| PMF | 0.09 | 0.16 | 0.04 | 0.77 | 0.15 | 0.28 | 0.76 | 0.15 | 0.41 | 0.01 | |
| Verify score | -0.46 | 0.11 | -0.39 | 0.31 | 0.51 | 0.31 | 9.0 | 0.31 | 0.36 | -0.03 | |
| PSI- BLAST | 0.0042 | 5.10E-33 | 0.0098 | 0.0012 | 0.007 | 1.70E-48 | 5.10E-72 | 6.80E-63 | 8.50E-64 | 1.70E-61 | 1.40E-84 |
| End AA | 618 | 718 | 628 | 481 | 499 | 405 | 200 | 155 | 665 | 639 | 499 |
| Start AA | 158 | 351 | 158 | 225 | 341 | . 167 | 181 | 220 | 282 | 330 | 129 |
| Chain ID | | Ą | Ą | V | ٧ | ٧ | ¥ | Ą | A | ٧ | æ |
| EOB EO | la7i | 1589 | lexx | Icrz | lorz | Ē | lerj | lerj | lerj | lerj | lgot |
| SEQ NO: | 459 | 459 | 459 | 465 | 465 | 465 | 465 | 465 | 465 | 465 | 465 |

| PDB annotation | COMPLEX (GTP. BINDINGTRANSDUCER) BETA1, TRANSDUCIN BETA SUBJUIT; GAMAAI, TRANSDUCIN GAMAA SUBJUIT; COMPLEX (GTP. BINDINGTRANSDUCER), G PROTEIN, HETEROTRINIER S SIGNAL | COMPLEX (GTP. BINDINGTRANSDUCER,) BETA1, TRANSDUCTN BETA SUBINIT; GAMMAI, TRANSDUCTN GAMMA SUBUNIT; COMPLEX (GTP. BINDINGTRANSDUCER), G PROTEIN, HETEROTRINER 2 SIGNAL | OXIDOREDUCTASE ENZYME, NIRTUR ERBUCTASE, OXIDOREDUCTASE, DENITRIFICATION, 2 ELECTRON TRANSPORT, PERIPLASMIC | TRANSFERASE ESAI HAT, ESAI PROTEIN, ESAIP, HISTONE ACETYLTRANSFERASE, COENZYME A | TRANSFERASE TRANSFERASE (PHOSPHORYL) | TRANSFERASE TRANSFERASE (PHOSPHORYL) | | |
|------------------|--|--|---|---|--|--|--|---|
| Coumpound | GT-ALPHA/GI-ALPHA CHMERA; CHAIN: A; GT- BETA; CHAIN: B; GT- GAMMA; CHAIN: G; | GTALPHAGIALPHA CHIMERA, CHANI: A; GT- BETA; CHANI: B; GT- GAMMA; CHANI: G; | CYTOCHROME CDI NITRITE REDUCTASE; CHAIN: A, B; | ESAI HISTONE ACETYLTRANSFERASE; CHAIN: A; | PHOSPHOGLYCERATE MUTASE: CHAIN: A. B: | PHOSPHOGLYCERATE MUTASE; CHAIN: A, B; | TRANSFERASE (PHOSPHORYL) PHOSPHOGLYCERATE MUTASE (E.C.2.7.5.3) DE- PHOSPHO ENZYME 3PGM 4 | TRANSFERASE (PHOSPHORYL) PHOSPHOGLYCERATE PHOSPHO EC.2.7.5.3) DE- PHOSPHO ENZYME 3PGM 4 |
| SeqFold score | | | | | 238.98 | | | 226.92 |
| PMF | 0.93 | 0.13 | 0.37 | 1 | | _ | _ | |
| Verify score | 0.57 | 0.28 | 0.2 | 9.6 | | 68:0 | 0.51 | |
| PSI- BLAST | 1.40E-84 | 8.50E-64 | 4.20E-36 | 0 | 6.80E-75 | 6.80E-75 | 7.00E-75 | 7.00E-75 |
| End | 499 | 639 | 498 | 290 | 257 | 259 | 249 | 250 |
| Start | | 326 | 167 | 17 | 16 | 16 | 16 | 91 |
| Chain | Д | m · | ∢ | V V | V | < | | |
| E CE | 1got | lgot | 1qks | 15,7 | lqhf | Iqhf | 3pg m | 3pg m |
| Se Se | 465 | 465 | 465 | 468 | 470 | 470 | 470 | 470 |

| | | | | | | | | | |
|----------------|---|--|---|--|---|---|---|---|---|
| PDB annotation | | TRANSCRIPTION REGULATION PROTO-ONCOGENE, NUCLEAR BODIES (PODS), LEUKEMIA, 2 TRANSCRIPTION REGULATION | | | LIGASE CBL, UBCH7, ZAP-70, E2, UBIQUITINE, B.; PHOSPHORYLATION, 2 TYROSINE KINASE, UBIQUITINATION, PROTEIN DEGRADATION, | LIGASE CBL, UBCH7, ZAP-70, E2, UBQUTIN, B3, PAGSPHOKYLATION, 2 TYROSINE KINASE, UBIQUITINATION, PROTEIN DEGRADATION, | METAL BINDING PROTEIN RING FINGER PROTEIN MATI; RING FINGER (C3HC4) | METAL BINDING PROTEIN RING FINGER PROTEIN MAT1; RING FINGER (C3HC4) | DNA-BINDING PROTEIN V(D)J RECOMBINATION ACTIVATING PROTEIN I; RAGI, V(I)J RECOMBINATION, ANTIBODY, MAD, RING FINGRR, 2 ZING BINUCLEAR |
| Coumpound | TRANSFERASE (PHOSPHORYL) PHOSPHOGLYCERATE MUTASE (E.C.2.7.53) DE- PHOSPHO ENZYME 3PGM 4 | TRANSCRIPTION FACTOR PML; CHAIN: NULL; | VIRUS EQUINE HERPES VIRUS-1 (C3HC4, OR RING DOMAIN) ICHC 3 (NMR, 1 STRUCTURE) ICHC 4 | VIRUS EQUINE HERPES VIRUS-1 (C3HC4, OR RING DOMÁRN) ICHC 3 (NMR, 1 STRUCTURE) ICHC 4 | SIGNAL TRANSDUCTION PROTEIN CBL; CHAIN: A; ZAP-70 PEPTIDE, CHAIN: B; UBIQUITIN-CONJUGATING ENZYME E12-18 KDA UBCH7; CHAIN: C; | SIGNAL TRANSDÜCTION PROTEIN CBL; CHAIN: A; ZAP-10 PEPTIDE; CHAIN: B; UBIQUITIN-CONJUGATING ENZYME E12-18 KDA UBCH7; CHAIN: C; | CDK-ACTIVATING KINASE ASSEMBLY FACTOR MATI; CHAIN: A: | CDK-ACTIVATING KINASE ASSEMBLY FACTOR MATI; CHAIN: A: | RAGI; CHAIN: NULL; |
| SeqFold | | | | | | | | | |
| PMF score | _ | 0.04 | 96.0 | 99:0 | 0.51 | 9.6 | 0.71 | 0.43 | 0.93 |
| Verify | 0.72 | -0.13 | 0.11 | -0.45 | -0.26 | -0.36 | -0.15 | 0.21 | -0.05 |
| PSI- BLAST | 1.50E-67 | 3.40E-07 | 5.60E-12 | 1.70E-11 | 8.40E-14 | 1.70E-11 | 5.60E-13 | 3.40E-06 | 2.80E-25 |
| End | 251 | 70 | 13 | 92 | 11 | 11 | 73 | 08 | 112 |
| Start | 16 | 1.7 | | 29 | 27 | 29 | 28 | 29 | 20 |
| Chain | | | | | 4 | Ą | ¥ | ¥ | |
| PDB ID | 3pg m | Ibor | Ichc | 1chc | 1fbv | Ifbv | 1g25 | 1825 | Irmd |
| SEQ US EQ | 470 | 473 | 473 | 473 | 473 | 473 | 473 | 473 | 473 |

| PDB annotation | CLUSTER, ZINC FINGER, DNA- BINDING PROTEIN | DNA-BINDING PROTEIN V(D)J RECOMBINATION ACTIVATING PROTEIN 1: RAGI V(D)J | RECOMBINATION, ANTIBODY, MAD, RING FINGER, 2 ZINC BINUCLEAR | CLUSTER, ZINC FINGER, DNA- BINDING PROTEIN | DNA-BINDING PROTEIN V(D)J RECOMBINATION ACTIVATING PROTEIN I: RAGI V(D)J | RECOMBINATION, ANTIBODY, MAD, RING FINGER, 2 ZINC BINUCLEAR | CLUSTER, ZINC FINGER, DNA- BINDING PROTEIN | COMPLEX (TRANSCRIPTION PEGIT ATTOMONA) VING VANG 1. | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | | LIPID TRANSPORT APO A-1; LIPOPROTEIN, LIPID TRANSPORT, CHOLESTEROL METABOLISM, 2 ATHEROSCLEROSIS, HDL, LCAT- | STRUCTURAL PROTEIN TWO PERFATS OF SPECTRIN AT PHA | HELICAL LINKER REGION, 22 TANDEM 3-HELIX COILED-COILS, | STRUCTURALTROTEIN | |
|-----------------|---|--|---|---|--|--|---|---|---------------------------|---|--------------------------------|---|--|---|--|-------------------|---|
| Coumpound | | RAGI; CHAIN: NULL; | | | RAGI; CHAIN: NULL; | | | YY1; CHAIN: C; ADENO- | INITIATOR ELEMENT DNA; | CHAIN: A. B; | | ZINC FINGER DNA BINDING DOMAIN ZINC-FINGER (ZFY- 6T) (NMR, 13 STRUCTURES) 5ZNF 3 | APOLIPOPROTEIN A-I; CHAIN: A, B, C, D; | ALPHA SPECTRIN; CHAIN: | S G G | DNA-BINDING HIGH | MOBILITY GROUP PROTEIN FRAGMENT-B (HMGB) |
| SeqFold | | | | | 54.37 | | | | | | | | 61.09 | 51.86 | | | |
| PMF | | 0.86 | | | | | | 90.0 | | | | 0.12 | | | | 10:0 | |
| Verify score | | -0.26 | | | | | | -0.51 | | | | -0.67 | | | | -0.45 | |
| PSI- BLAST | | 5.10E-21 | | | 2.80E-25 | | | 3.40E-11 | | | | 0.0042 | 0.00056 | 0.00098 | | 0.0014 | |
| End | | 114 | | | 114 | | | 194 | | | | 167 | 206 | 219 | | 204 | |
| Start | | 23 | | | 7 | | | 68 | | | | 140 | - | 13 | | 164 | |
| Chain | | | | | | | | U | | | | | V | V. | | | |
| ag a | | 1md | | | Imd | | | Inpq | | | | 5znf | lavi . | lcun | | 1hm | e |
| SEQ NO: | | 473 | | | 473 | | | 473 | | | | 473 | 475 | 475 | | 475 | |

| | | | | | | | | | | | | _ |
|-----------------|--|---|--|---|---|---|---|---|---|---|---|--------------------------|
| PDB annotation | | | CONTRACTILE PROTEIN TRIPLE. HELIX COILED COIL, CONTRACTILE PROTEIN | CHAPERONE HSP40, CHAPERONE, HEAT SHOCK, PROTEIN FOLDING, DNAK | CHAPERONE HSP40; CHAPERONE, HEAT SHOCK, PROTEIN FOLDING, DNAK | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELICAL REPEAT HSP90. 2 PROTEIN BINDING | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELICAL REPEAT, HSC70, 2 HSP70, PROTEIN BINDING | SIGNALING PROTEIN PEROXISMORE RECEPTOR 1, PTSI-BP, PEROXIN-5, PTSI PROTEIN-PERTIDE COMPLEX, TETRATRICOPEPTIDE REPEAT, TPR, 2 HELICAL REPEAT | MOLECULAR CHAPERONE HDJ-1; MOLECULAR CHAPERONE | MOLECULAR CHAPERONE HDJ-1; MOLECULAR CHAPERONE | MOLECULAR CHAPERONE HDJ-1; MOLECULAR CHAPERONE | CALCIUM-BINDING CALCIUM- |
| Coumpound | (DNA-BINDING 1HME 3 HMG-BOX DOMAIN B OF RAT HMGI) (NMR, 1 STRUCTURE) 1HME 4 | DNA-BINDING HIGH MOBILITY GROUP PROTEIN I (FMGI) BOX 2, COMPLEXED WITH 1HSM 3 MERCAPTOETHANOL (NMR, MINIMIZED AVERAGE | STRUCTURE) 1HSM 4 HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A. | DNAJ; CHAIN: NULL; | DNAJ; CHAIN: NULL; | TPR2A-DOMAIN OF HOP; CHAIN: A; HSP90-PEPTIDE MEEVD: CHAIN: B: | TPRI-DOMAIN OF HOP; CHAIN: A, B; HSC70- PEPTIDE; CHAIN: C, D; | PEROXISOMAL TARGETING SIGNAL I RECEPTOR; CHAIN: A, B; PTS1- CONTAINING PEPTIDE; CHAIN: C, D; | HUMAN HSP40; CHAIN: NULL; | HUMAN HSP40; CHAIN: NULL; | HUMAN HSP40; CHAIN: NULL; | NEUROCALCIN DELTA; |
| SeqFold | | | 55.34 | 72.19 | | | | | | 80.39 | | |
| PMF | | 0.12 | | | _ | -0.09 | 0.05 | -0.02 | _ | | _ | 0.39 |
| Verify score | | -0.39 | | | 11:1 | 0.38 | 0.42 | 0 | 1.05 | | 0.98 | -0.35 |
| PSI- BLAST | | 0.00084 | 4.20E-08 | 1.20E-19 | 1.20E-19 | 1.20E-19 | 8.50E-24 | 1.00E-18 | 1.20E-19 | 1.40E-30 | 1.40E-30 | 0.00013 |
| End | | 210 | 222 | 182 | 181 | 129 | 123 | 801 | 180 | 187 | 176 | 92 |
| Start | | 164 | | 801 | 110 | 9 . | 9 | 7 | 107 | 107 | 109 | 43 |
| Chain | | | 4 | | | ∢ | < | * | | | | ¥ |
| EQ O | | Ihsm | nnbj | 1bq0 | 1bq0 | ler | lelw | . Igh | Ihdj | 1hdj | lhdj | Jiq. |
| SEQ NO B | | 475 | 475 | 477 | 477 | 477 | 477 | 477 | 477 | 477 | 477 | 419 |

| | | | | | | | | | | | _ |
|------------------|--|--|---|---|--|---|--|---|---|---|---|
| PDB annotation | BINDING, MYRISTOYLATION, NEURONAL SPECIFIC GUANYLATE 2 CYCLASE ACTIVATOR | SIGNALING PROTEIN CALCIUM BINDING, SIGNALING DOMAIN, NPF BINDING, FW BINDING, 2 EF-HAND, EH DOMAIN, SIGNALING PROTEIN | METAL BINDING PROTEIN CAVP; EF- HAND FAMILY, CALCIUM BINDING PROTEIN, NMR | | - | STRUCTURAL PROTEIN HELIX-TURN- HELIX | METAL TRANSPORT CALMODULIN, HIGH RESOLUTION, DISORDER | METAL BINDING PROTEIN YEAST FREQUENIN EF-HAND, CALCIUM | CALCIUM-BINDING PROTEIN CALCIUM-MYRISTOYL SWITCH, CALCUIM-BINDING PROTEIN | GENE REGULATION POZ DOMANN. PROFIEM-RPROTEN INTERACTION DOMAN, TRANSCRIPTIONAL 2 REPRESOR, ZINC-ENGER PROTEN, X.AAY CRYSTALLOGAPHY, 3 PROTEN STRUCTURE, PROAFFACTIC LEUKEMIA, GENE REGULATION | LIGASE CYCLIN A/CDK2- ASSOCIATED PROTEIN P45; CYCLIN A/CDK2-ASSOCIATED PROTEIN P19; |
| Coumpound | CHAIN: A, B; | EPIDERMAL GROWTH FACTOR RECEPTOR PATHWAY CHAIN: A; | CALCIUM VECTOR PROTEIN; CHAIN: A; | CALCIUM-BINDING PROTEINC ALAMODULIN COMPLEXED WITH CALMODULIN-BINDING DOMAIN OF ICDM 3 CALMODULIN-BEPENDENT ROTEIN KINASE II ICDM 4 | CALCIUM-BINDING PROTEIN CALMODULIN (VERTEBRATE) ICLL 3 | CARDIAC TROPONIN C; CHAIN: A; | CALMODULIN; CHAIN: A; | CALCIUM-BINDING PROTEIN NCS-1; CHAIN: A; | RECOVERIN; CHAIN: NULL; | PROMYELOCYTIC LEUKEMIA ZINC FINGER PROTEIN PLZF, CHAIN: A; | SKP2; CHAIN: A, C, B, G, I, K, M, O; SKP1; CHAIN: B, D, F, H, J, L, N, P; |
| SeqFold score | | | | | | | | | | | |
| PMF | | 0.92 | 0.42 | 0.51 | 0.13 | 0.12 | 0.27 | 0.21 | 0.05 | 0.63 | . 69:0 |
| Verify score | | -0.18 | -0.3 | 0.54 | 0.07 | 0.28 | 60:00 | 0.14 | -0.43 | 0.11 | -0.06 |
| PSI- BLAST | | 0.00014 | 0.00028 | 8.40E-05 | 4.20E-05 | 0.00017 | 0.00014 | S.60E-05 | 0.00028 | 1.70E-24 | 1.10E-05 |
| End | | 83 | 83 | | 103 | 8 | 103 | 8 | 96 | 143 | 168 |
| Start | | 41 | 14 | 41 | 41 | 43 | 14 | 43 | 42 | 22 | 52 |
| Chain | | A | V | ¥ | | ۷ | ¥ | ⋖ | | V | В |
| 10B | | 1c07 | 1c7w | рот ш | lel | 墨 | lexr | lfpw | liku | 1buo | lfqv |
| SE SE | | 479 | 479 | 479 | 479 | 479 | 479 | 479 | 479 | 480 | 480 |

| | | | | | | | _ | | | | |
|------------------|--|---|--|--|--|--|---|---|--|---|---|
| PDB annotation | SKPI, SKP2, F-BOX, LRR, LEUCINE- RICH REPEAT, SCF, UBIQUITIN, 2 E3, UBIQUITIN PROTEIN LIGASE | LIGASE SKP2 F-BOX; SKP1; SKP1, SKP2, F-BOX, LRR, LEUCINE-RICH REPEAT, SCF, UBIQUITIN, 2 E3, UBIQUITIN PROTEIN LIGASE | LIGASE CYCLIN A/CDK2- ASSOCIATED P45; CYCLIN A/CDK2- ASSOCIATED P19; SKP1, SKP2, FBOX, LRRS, LEUCINE-RICH REPEATS, SCF, 2 UBRQUITIN, E3, UBRQUITIN PROTEIN LIGASE | · | | | | INSECT IMMUNITY INSECT IMMUNITY, LPS-BINDING, HOMOPHILIC ADHESION | GROWTH FACTOR/GROWTH FACTOR RECEITOR FGE, FOFF, IMMUNGGLOBULIN-LIKE, SIGNAL TRANSDUCTION, 2 DIMERIZATION GROWTH FACTOR/GROWTH FACTOR RECEITOR | VIRUSVIRAL PROTEIN, RECEPTOR CD155, PVR, HUMAN POLIOVIRUS, ELECTRON MICROSCOPY, 2 POLIOVIRUS-RECEPTOR COMPLEX, VIRUSVIRAL PROTEIN, RECEPTOR | GROWTH FACTOR/GROWTH FACTOR RECEPTOR FGF2; FGFR2; IMMUNOGLOBUL/N (IG)LIKE |
| Coumpound | | CYCLIN A/CDK2- ASSOCIATED P19; CHAIN: A, C; CYCLIN A/CDK2- ASSOCIATED P45; CHAIN: B, D; | SKP2; CHAIN: A, C; SKP1; CHAIN: B, D; | OXIDOREDUCTASE(OXYGE N(A)) GALACTOSE OXIDASE (E.C.1.1.3.9) (PH 4.5) 1GOF 3 | OXIDOREDUCTASE(OXYGE N(A)) GALACTOSE OXIDASE (E.C.1.1.3.9) (PH 4.5) 1GOF 3 | OXIDOREDUCTASE(OXYGE N(A)) GALACTOSE OXIDASE (E.C.1.1.3.9) (PH 4.5) 1G0F 3 | | HEMOLIN; CHAIN: A, B; | FIBROBLAST GROWTH FACTOR 2; CHAIN: A, B; FIBROBLAST GROWTH FACTOR RECEPTOR 1; CHAIN: C, D; | POLIOVIRUS RECEPTOR; CHAIN: R; VP1; CHAIN: 1; VP2; CHAIN: 2; VP3; CHAIN: 3; VP4; CHAIN: 4; | FIBROBLAST GROWTH FACTOR 2; CHAIN: A, B, C, D; FIBROBLAST GROWTH |
| SeqFold | | | | | | | | | | | |
| PMF | | 0.96 | 0.86 | -0.08 | 0.22 | -0.18 | | -0.17 | 0.21 | -0.14 | 0.17 |
| Verify score | | 0.48 | 0.26 | 0.22 | 0.31 | 0.07 | | 0 | -0.04 | 0.03 | 0.05 |
| PSI- BLAST | | 4.20E-05 | 0.00042 | 1.40E-31 | 8.50E-13 | 2.80E-14 | | 1.70E-29 | 1.405-12 | 1.70E-14 | 5.10E-13 |
| End | | 141 | 164 | 21.5 | 288 | 592 | | 396 | 396 | 381 | 392 |
| Start AA | | 52 | 22 | 318 | 346 | 362 | | 66 | 303 | 96 | 303 |
| Chain ID | | g | В | | | | | ¥ | Q | Я | a |
| PDB ID | | lfsi | 162 | lgof | lgof | lgof | | 1bih | lcvs | Idgi | lev2 |
| SEQ ID NO: | | 480 | 480 | 480 | 480 | 480 | | 481 | 481 | 481 | 481 |

| PDB annotation | DOMAINS BELONGING TO THE I-SET 2 SUBGROUP WITHIN IG-LIKE DOMAINS, B-TREFOIL FOLD | GROWTH FACTOR/GROWTH FACTOR RECEPTOR FOFF, GRFZ; INAUTNOGLOBULIN (IG)LIKE DOMAINS BELONGING TO THE I-SET S SUBGROUP WITHIN IGLIKE DOMAINS, B-TREFOIL FOLD | GROWTH FACTORGROWTH FACTOR RECEPTOR FOGT, IGENT, IMMUNOGLOBULIN (IG) LIKE DOMANNS BELONGING TO THE I-SET S UBGROUP WITHIN IG-LIKE DOMANNS, B-TREFOLL FOLD | IMMUNE SYSTEM FC-EPSILON RI- ALPHA; IMMUNOGLOBULIN FOLD, GLYCOPROTEIN, RECEPTOR, IGE- BINDING 2 PROTEIN | CONTRACTILE PROTEIN IMMUNOGLOBULIN FOLD, BETA BARREL | KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION | IMMUNE SYSTEM CD32; RECEPTOR, FC, CD32; IMMUNE SYSTEM | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELICAL REPEAT, HSP90, 2 PROTEIN BINDING | HALOPEROXIDASE HALOPEROXIDASE F; HALOPEROXIDASE F; HALOPEROXIDASE, COMPLEX COMPLEX COMPLEX | HYDROLASE BPHD; HYDROLASE, PCB DEGRADATION | HYDROLASE PNB ESTERASE; ALPHA- BETA HYDROLASE, DIRECTED |
|-----------------|--|---|---|--|--|--|---|--|--|---|--|
| Coumpound | FACTOR RECEPTOR 2; CHAIN: E, F, G, H; | FIBROBLAST GROWTH FACTOR 2; CHAIN: A, B, C, D; FIBROBLAST GROWTH FACTOR RECEPTOR 2; CHAIN: E, F, G, H; | FIBROBLAST GROWTH FACTOR I; CHAIN: A, B; FIBROBLAST GROWTH FACTOR RECEPTOR 1; CHAIN: C, D; | HIGH AFFINITY INMUNOGLOBULIN EPSILON RECEPTOR CHAIN: A; | TELOKIN; CHAIN: A | TWITCHIN; CHAIN: NULL; | FC GAMMA RIIB; CHAIN: A; | TPRZA-DOMAIN OF HOP; CHAIN: A; HSP90-PEPTIDE MEEVD; CHAIN: B; | CHLOROPEROXIDASE F; CHAIN: NULL; | 2-HYDROXY-6-OXO-6- PHENYLHEXA-2,4- DIENOATE CHAIN: A: | PARA-NITROBENZYL ESTERASE, CHAIN: A; |
| SeqFold | | | | | | | | | | | |
| PMF | | 0.15 | 0.1 | 90.04 | -0.07 | 0.03 | 10:0 | 0.09 | 0.04 | 0.47 | _ |
| Verify score | | -0.2 | 0.02 | -0.2 | 0.13 | 90.0 | -0.06 | 90:0- | 0.45 | 0.29 | 0.39 |
| PSI- BLAST | | 5.10E-13 | 1.40E-12 | 1.70E-16 | 3.40E-17 | 8.50E-16 | 1.70E-14 | 0.00014 | 0.0017 | 0.00012 | 3.40E-93 |
| End | | 392 | 396 | 386 | 381 | 382 | 384 | 363 | 296 | 331 | 909 |
| Start | | 303 | 303 | 261 | 589 | 292 | 161 | 281 | | 178 | 43 |
| Chain D | | ڻ ت | U | ¥ | ∢ | | 4 | 4 | | < | V |
| PDB 03 | | lev2 | levt | pāl | Iffig. | Ikoa | 2fcb | Icfr | la8s | Ic4x | lc7j |
| SEQ B B S | | 481 | 481 | 184 | 481 | 481 | 481 | 482 | 483 | 483 | 483 |

| | | | , | , | | | | | | , | |
|----------------|---|---|--|--|--|---|--|--|--|---|--|
| PDB annotation | EVOLUTION, ORGANIC ACTIVITY, 2 PNB ESTERASE | LIPASE ESTERASE, SUBSTRATE/PRODUCT-BOUND ICLE 9 | LPASE ESTERASE, SUBSTRATE/PRODUCT-BOUND ICLE 9 | HYDROLASE LINB, 1,3,4,6- TETRACHLORO-1,4- CYCLOHEXADIENE DEHALOGENASE, LINDANE, BIODEGRADATION, ALPHANBETA-HYDROLASE | HYDROLASE (SERIME ESTERASE) HYDROLASE (SERIME ESTERASE), HYDROLASE, SERIME ESTERASE, STRAKES, MEMBRANE, NERVE, MUSCLE, SIGNAL, NEJROTORANBAITTERR DEGRADATION, GLYCOPROPE OPPLANCHOR, ALTERNATIVE SPLICING | CHOLINESTERASE SERINE HYDROLASE, NEUROTRANSMITTER CLEAVAGE, CATALYTIC 2 TRIAD, ALPHA/BETA HYDROLASE | HYDROLASE ALPHA/BETA HYDROLASE FOLD | HYDROLASE ALPHA/BETA HYDROLASE FOLD | HYDROLASE BILE SALT ACTIVATED LIPASE, ESTERASE, CATALYTIC DOMAIN | SERINE HYDROLASE SERINE HYDROLASE, DEGRADATION OF BREFELDIN A, ALPHA'BETA 2 HYDROLASE FAMILY | |
| Coumpound | | CHOLESTEROL ESTERASE; ICLE 4 CHAIN: A, B; ICLE 5 | CHOLESTEROL ESTERASE; ICLE 4 CHAIN: A, B; ICLE 5 | HALOALKANE DEHALOGENASE, CHAIN: A; | ACETYLCHOLNESTERASE, CHAIN: A; | ACETYLCHOLINESTERASE; CHAIN: A; | SERINE HYDROLASE; CHAIN: A; | SERINE HYDROLASE; CHAIN: A; | BILE SALT ACTIVATED LIPASE; CHAIN: A; | BREFELDIN A ESTERASE; CHAIN: A, B; | HYDROLASE LIPASE (B.C.3.1.1.3) (TRIACYLGLYCEROL LIPASE) COMPLEXED WITH |
| SeqFold | | 181.19 | | | | | | | | | 179.92 |
| PMF score | | | ı | 0.57 | - | _ | 0.58 | 0.42 | | 0.1 | |
| Verify | | | 0.21 | 9.0 | 0.61 | 0.59 | 0.17 | -0.05 | 5.0 | -0.05 | |
| PSI- BLAST | | 1.20E-73 | 1.20E-73 | 0.0084 | 0 | 0 | 3.40E-28 | 5.60E-39 | 0 | 5.10E-20 | 1.20E-71 |
| End | | 185 | 293 | 379 | 611 | 612 | 346 | 283 | 612 | 334 | 581 |
| Start AA | | 42 | 89 | 163 | 40 | 40 | 142 | 73 | 44 | 88 | 42 |
| Chain | | V | ¥. | ¥ | ₹ | ∢ | V | A | ¥ | × | |
| PDB CD | | lcle | lcle | 1cv2 | 1dx4 | lea5 | levq | levq | 1f6w | 1 jkm | Ilpp |
| SEQ B B S | | 483 | 483 | 483 | 483 | 483 | 483 | 483 | 483 | 483 | 483 |

| | | | | | | | | | | _ | | | | | | | | | | | | _ | | | | | _ | |
|--|---|------------------|---------------|------------------------|--------|------------------------------------|---|---|--|-----------------------------|--------------------|-----------------------|----------------------|--------------------------------|-----------------------------------|--------------------------------|-----------------------|------------------------|---|--------------------------|------------------------------|-----------|------------------------|--|--------------------------|------------------------------|------------------|---|
| PDB annotation | | | | · | | | HYDROLASE MACHE, HYDROLASE, SERINF ESTERASE | ACETYLCHOLINESTERASE, | TETRAMER, 2 HYDROLASE FOLD, GLYCOSYLATED PROTEIN | HYDROLASE MACHE; HYDROLASE, | SERINE ESTERASE, | ACETYLCHOLINESTERASE, | GLYCOSYLATED PROTEIN | HYDROLASE PNB ESTERASE; ALPHA- | BETA HYDROLASE DIRECTED EVOLUTION | HYDROLASE PNB ESTERASE; ALPHA- | EVOLUTION | HYDROLASE PROLYL | ENDOPEP I IDASE, POST-PROLINE OF FAVING PROF VI | OLIGOPEPTIDASE, AMNESIA, | ALPHA/BETA-HYDROLASE, BETA-2 | PROPELLER | HYDROLASE PROLYL | ENDOPEPTIDASE, POST-PROLINE CLEAVING PROLYT. | OLIGOPEPTIDASE, AMNESIA, | ALPHA/BETA-HYDROLASE, BETA-2 | LINOLETICEN | |
| Coumpound | 1LPP 3 HEXADECANESULFONATE 1LPP 4 1LPP 71 | HYDROLASE LIPASE | (E.C.3.1.1.3) | LIPASE) COMPLEXED WITH | 1LPP 3 | HEXADECANESULFONATE ILPP 4 ILPP 71 | ACETYLCHOLINESTERASE; | 6 | | ACETYLCHOLINESTERASE; | CHAIN: A, B, C, D; | | | PARA-NITROBENZYL | ESTERASE; CHAIN: A; | PARA-NITROBENZYL | bottempt, circuit. A, | PROLYL OLIGOPEPTIDASE; | CHAIN: A; | | | | PROLYL OLIGOPEPTIDASE; | CHAIN: A: | | | OF PROCEED SOUTH | HYDROLASE(CARBOXYLIC ESTERASE) LIPASE (E.C.3.1.1.3) |
| SeqFold | | | | | | | 368.25 | | | | | | | 242.59 | | | | | | | | | | | | | . 0.0 | 710.1 |
| PMF | | _ | | | | | | | | _ | | | | | | _ | | 0.11. | | | | | 0.03 | | | | | |
| Verify score | | 0.22 | | | | | | | | 0.72 | | | | L | | 0.33 | | 0.15 | | | | | 0 | | | | | |
| PSI- BLAST | | 1.20E-71 | | | | | 0 | | | 0 | | | | 1.70E-89 | | 1.70E-89 | | 5.60E-57 | | | | | 1.20E-35 | | | | 6 100 00 | 5.10E-80 |
| End | | 593 | | | | | 612 | | | 612 | | _ | | 602 | | 599 | | 397 | | | | 5 | 320 | | | | 50,5 | 080 |
| Start | | 89 | | | | | 38 | | | 38 | | | | 40 | | 43 | | 56 | | | | | 82 | | | | | 9 |
| Chain ID |) | | | | | | ٧ | | | A | | | | ¥ | | ٧ | | ٧ | | | | | < | | | | | |
| EDB EDB | | di. | | | | | Ітаа | | | 1 maa | | | | 1qe3 | | Iqe3 | | lqfm | | | | | mgb. | | | | | g 5 |
| Sa Si Si Si Si Si Si Si Si Si Si Si Si Si S | | 483 | | | | | 483 | | | 483 | | | | 483 | | 483 | | 483 | | | | 5 | 483 | | | | 163 | 483 |

| | | | | | | | | _ | | | | |
|----------------|-------------------------------------|---|--|--|---|--|---|---|---|---|---|--|
| PDB annotation | | | HYDROLASE BILE SALT ACTIVATED LIPASE, BILE SALT STIMULATED HYDROLASE, SERINE ESTERASE, LIPASE | HYDROLASE BILE SALT ACTIVATED LIPASE, BILE SALT STIMULATED HYDROLASE, SERINE ESTERASE, LIPASE | HEXOKINASE ATP/.D-HEXOSE-6- PHOSPHOTRANSFERASE; HEXOKINASE, PHOSPHOTRANSFERASE | HEXOKINASE ATP:D-HEXOSE-6- PHOSPHOTRANSFERASE; HEXOKINASE. PHOSPHOTRANSFERASE | TRANSFERASE STRUCTURALLY HOMOLOGOUS DOMAINS | | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER,DNA) COMPLEX (ZINC FINGER,DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA |
| Coumpound | TRIACYLGLYCEROL HYDROLASE 1THG 3 | HYDROLASE(CARBOXYLIC ESTERASE) LIPASE (E.C.3.11.3) TRIACYLGIYCEROL HYDROLASE ITHG 3 | CHOLESTEROL ESTERASE; CHAIN: NULL; | CHOLESTEROL ESTERASE; CHAIN: NULL; | HEXOKINASE; CHAIN: A, B; | HEXOKINASE; CHAIN: A, B; | HEXOKINASE TYPE I; CHAIN: N; | | QGSR ZINC FINGER PEPTIDE, CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER |
| SeqFold | | | 318.91 | | | 179.92 | | | | | | |
| PMF | | _ | | - | - | | _ | | 0.11 | 0.3 | 0.94 | 0.11 |
| Verify | | 0.49 | | 0.54 | 1.19 | | 1.21 | | -0.49 | -0.36 | 0.16 | -0.34 |
| PSI- BLAST | | 5.10E-80 | 0 | 0 | 0 | 0 | 0 | | 1.70E-18 | 1.70E-23 | 6.80E-24 | 1.70E-30 |
| End | | 283 | 819 | 612 | 910 | 116 | 913 | | 204 | 232 | 260 | 204 |
| Start | | 47 | 33 | 44 | - | - | 16 | | 127 | 152 | 180 | 126 |
| Chain ID | | | | | ¥ | ¥ | z | | ∢ | 4 | ∀ | ပ |
| 20g CE | | Ithg | 2bce | 2bce | lbg3 | 1bg3 | lcza | | lalh | laih | lalh | lme y |
| SEQ BO | | 483 | 483 | 483 | 484 | 484 | 484 | | 485 | 485 | 485 | 485 |

| PDB annotation | INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 RYSTAL STRUCTINE, COMPLEX | COMPLEX (ZINC FINGERDNA) ZINC COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DINA) ZINC FINGER, PROTEIN-DINA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DINA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 |
|------------------|---|---|---|--|--|--|--|---|---|
| Coumpound | PROTEIN, CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN; A, B, D, E; CONSENSUS ZINC PINCER PROTEIN; CHAIN; C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; |
| SeqFold score | | | | · | | | | | |
| PMF | | 0.69 | 0.99 | _ | _ | _ | _ | _ | |
| Verify score | | -0.18 | -0.01 | 0.05 | 0.27 | 0.25 | 0.25 | 0.67 | 0.67 |
| PSI- BLAST | | 5.10E-38 | 8.50E-41 | 1.20E-42 | 1.40E-43 | 2.80E-47 | 5.10E-47 | 1.50E-48 | 2.80E-51 |
| End AA | ı | 232 | 260 | 288 | 316 | 372 | 372 | 400 | 400 |
| Start | | 151 | 179 | 207 | . 235 | 291 | 291 | 319 | 319 |
| Chain | | v. | o | ပ | O | ပ | ပ | ပ | ပ |
| 808 E | | J me | Ime y | Jme y | Ime y | Ime y | J me | lme Y | y me |
| SEQ B SEQ | | 485 | 485 | 485 | 485 | 485 | 485 | 485 | 485 |

| PDB annotation | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX CANC FINGER DNA! | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX |
|-----------------|--|---|--|--|--|---|--|--|---|
| Coumpound | | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A. B, D, E. CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; |
| SeqFold | | | | | 113.26 | | | | |
| PMF score | | _ | _ | _ | | - | _ | _ | |
| Verify score | | 0.48 | 69:0 | 69:0 | | 0.41 | 0.05 | 0.02 | 0.1 |
| PSI- BLAST | | 5.10E-49 | 3.40E-49 | 4.20E-50 | 4.20E-50 | 1.00E-49 | 1.70E-50 | 1.50E-50 | 8.50E-51 |
| End | | 428 | 456 | 456 | 457 | 484 | 512 | 240 | 568 |
| Start AA | | 347 | 375 | 375 | 375 | 403 | 431 | 459 | 487 |
| Chain | | O | O | υ | ပ | ပ | ပ | v | c |
| PDB ED | | Ime y | y w | Jme y | Jme y | lme y | lme y | lme y | lme y |
| S e S | | 485 | 485 | 485 | 485 | 485 | 485 | 485 | 485 |

| | _ | | | | | | _ | _ | _ | | _ | | _ | | _ | | _ | | | | | | | | | | | | | | _ | _ | |
|------------------|-------------------|---|--|-------------------|--------------------------------|-----------------------|---------------------------|-------------------|--------------------------------|-----------------------|--------------------------------|--|--------------------------------|-----------------------|--------------------------------|----------------------------|-------------------|-----------------------|--------------------------------|----------------------------|-------------------|--------------------------------|----------------------|---------------------------|-------------------|-------------------------|-------------------------|----------------------|--------------------------------|---------------------------------|-------------------------|-------------------------|---|
| PDB annotation | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 CRYSTAL, STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-UNA | CRYSTAL STRUCTURE COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGENDINA) | FINGER, PROTEIN-DNA | INTERACTION. PROTEIN DESIGN. 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | PINGER, PROIEIN-DNA | CRYSTAL STRUCTURE COMPLEX | (ZINC FINGER/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX | REGILLATION/DNA) RNA | POLYMERASE III 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX | (TRANSCRIPTION RNA REGULATION/DNA), RNA |
| Coumpound | | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | DNA; CHAIN: A, B, D, E; | BOTTEN: CHAIN: C F C: | FROIEIN; CEMIN: C, F, G; | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, r, G; | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | Tale of the party | CONSENSUS ZINC FINGER | PROTEIN: CHAIN: C. F. G. | | | DNA; CHAIN: A, B, D, E; | PROTEIN: CHARL OF C. | ractein, chair. C. r. d. | | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL KNA GENE; | CEPALIN: B, C, E, F; | | | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | _ | | | 1 | | | | _ | | | | _ | | | | 1 | - | | | | 0.48 | | | | 0.76 | | | | | 0.81 | | |
| Verify score | | 0.02 | | | 0.03 | | | | 0.28 | | | | 0.15 | | | | ,,, | 200 | | | | -0.38 | | | | -0.28 | | | | | -0.2 | | |
| PSI- BLAST | | 1.50E-50 | | | 3.40E-50 | | | | 1.70E-50 | | | | 3.40E-50 | | | | 2000 | 1.00E-32 | | | | 5.10E-07 | | | | 3.40E-27 | | | | | 3.40E-31 | | |
| End AA | | 969 | | | 624 | | | | 652 | | | | 089 | | | | ,,, | G G | | | | 176 | | | | 274 | | | | | 297 | | |
| Start | | \$15 | | | 543 | | | | 57.1 | | | | 599 | | | | | /70 | | | | 149 | | | | 130 | | | | | 152 | | |
| Chain ID | | S | | | ၁ | | | | ၁ | | | | U | | | | , | - د | | | | _o | | | | ¥ | | | | | Ą | | |
| PDB DD | | y Inc | | | Ime | > | | | Ime | ^ | | | Ime | ^ | | | 1 |) III | | | | e i | <u>~</u> | | | 941 | | | | | 146 | | |
| SEQ NO: | | 485 | | | 485 | | | | 485 | | | | 485 | | | | 207 | | | | | 485 | | | | 485 | | | | | 485 | | |

| | | | | · | | | | _ | | | -7 | | | | | 7 | _ | _ | _ | | - | | | _ | _ | _ | _ |
|------------------|---|--|--|--|--|---|--------------------------|-------------------------|---|---------------------------------|---------------------------------|-------------------------|--------------------|----------------------|---------------------------------|---------------------------------|-------------------------|-----------------|----------------------|---------------------------------|---------------------------------|------------------------|--------------------------|--------------------------------|-----------------------------|------------------------|---|
| PDB annotation | POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION | REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX | (TRANSCRIPTION REGULATION/DNA), RNA | POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION . | REGULATION/DNA) COMPLEX | (IKANSCKIPTION REGIT ATTOMONA) RNA | POLYMERASE III, 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | CTRANSCRIPTION | REGULATION/DNA), RNA | POLYMERASE III, 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | TRANSCRIPTION | REGULATION/DNA), RNA | POLYMERASE III, 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (IKANSCRIPTION | TRANSCRIPTION INITIATION | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; |
| Coumpound | | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | | | TFIIIA; CHAIN: A, D; 5S | CHAIN: B. C. F. F. | | | | TFILIA; CHAIN: A, D; 5S | CHAIN: B C E F. | 5 | | Claret Court of the same | YYI; CHAIN: C; ADENO- | INITIATOR ELEMENT DNA: | CHAIN: A, B; | | | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 |
| SeqFold score | | | | 120.46 | | | | | | | | | | | | | | | | | | | | | | | |
| PMF score | | 1 | | | | | - | | | | | 66:0 | | | | | 0.99 | | | | 9 | 71.0 | | | | | 0.72 |
| Verify score | | 0.07 | | | | | 0.11 | | | | | 0.01 | | | | | 0.1 | | | | 000 | 77.77 | | | | | -0.27 |
| PSI- BLAST | | 6.80E-34 | | 5.10E-37 | | | 5.10E-37 | | | | | 3.40E-37 | | | | | 1.40E-36 | | | | 20.00.0 | 3.10E-23 | | | | | 8.50E-27 |
| End AA | | 353 | | 484 | | | 521 | | | | | 633 | | | | | 682 | | | | 22.0 | 767 | | | | | 260 |
| Start AA | | 208 | | 319 | | | 376 | | | | | . 488 | | | | | 244 | | | | 50 | /71 | | | | | 159 |
| Chain ID | | ٧ | | Ą | | | Ą | | | | | ٧ | | | | | ∢ | | | | , | | | | | | S |
| PDB DD | | 1116 | | 1 11 6 | | | 1116 | | | | , | £ | | | | 1 | £ | | | | 3 | 2001 | | | | | 1ubd |
| Se o | | 485 | | 485 | | | 485 | _ | | | | 482 | | _ | | 1 | £ | | | | 100 | ş | | | _ | | 485 |

| PDB annotation | TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULATIONDNA) TYRO-YAND I; TRANSCRIPTON INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROCIEN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REQUILATIONINNA) TYRG-YANO 1; TRANSCRIPTON INTIATION, INTIATIOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/NA) | COMPLEX (TRANSCRIPTION REGULATIONINNY) YMO-YMO 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDAA), | COMPLEX (TRANSCRIPTION REGULATIONINALY) YING-YANG I; TRANSCRIPTON INITIATION, INITIATOR BLEMENT, YYI, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDAN) | COMPLEX (TRANSCRIPTION - REGULATIONIN) THOSY AND !; TRANSCRIPTION INITIATION IN THAT THOSE SERVICE PROPERLY 174, ZINC 2 FINGER PROTEIN DNA-PROTEIN PRECOGNITION 3 COMPLEX RECOGNITION 3 COMPLEX | COMPLEX (TRANSCRIPTION |
|-----------------|---|---|--|--|--|---|------------------------|
| Coumpound | INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INTIATOR ELEMENT DNA; CHAIN: A, B; | YYI, CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED YIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B: | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YY1; CHAIN: C; ADENO- |
| SeqFold | | | | | | | |
| PMF | | 0.86 | 0.93 | - | 96:0 | - | _ |
| Verify score | | -0.04 | 0.32 | 0.18 | 0.02 | 0.14 | 0.63 |
| PSI- BLAST | | 3.40E-29 | 1.20E-29 | 8.50E-32 | 4.20E-46 | 7.00E-52 | 9.80E-59 |
| End | | 288 | 316 | 344 | 345 | 372 | 400 |
| Start AA | | 182 | 215 | 238 | 240 | 268 | 296 |
| Chain D | | ပ | ပ | ပ | U | U | ပ |
| EDB CD | · | lubd | Jubd | 1ubd | Jubd | Inpp | Inpd |
| Se Se Se | | 485 | 485 | 485 | 485 | 485 | 485 |

| PDB annotation | REGULATION/DNA) YING-YANG I; TRANSCRIPTON INITATION, INITATOR ELEMBRT, YY1, ZINC2 FINGER PROTEIN, DNA-PROTEIN RECOGNITEN, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-YANG I; TRANSCRIPTION INTIATION, INTIATIOR ELEMENT, YYI, ZENCZ FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONNA) | COMPLEX (TRANSCRIPTION REGULATIONDNA, YING-YANG I; TRANSCRIPTION INITIATION, MITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-YANG I; TRANSCRIPTION INITIATION, BITIATOR ELEMENT, YYI, ZING 2 FINGER PROTEIN DINA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGILATIONDNA) YING-YANG I; TRANSCRIPTON INTIATION, INTIATION BLEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-YANG I; TRANSCRIPTION INITIATION, INITIATION RELEMENT, YYI, ZINC 2 FINGER ROCTEIN DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX |
|-----------------|--|---|--|--|---|--|
| Coumpound | ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADBNO- ASSOCIATED VIRUS PS AINTIATOR ELEMENT DNA; CHAIN: A, B; | YY I; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INTIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A. B. |
| SeqFold | | | 100.22 | | | |
| PMF | | _ | | _ | - | _ |
| Verify score | | 3 0.0 | | 0.26 | 0.1 | 0:00 |
| PSI- BLAST | | 2.80E-59 | 2.80E-59 | 2.80E-55 | 8.40E-56 | 4.20E-59 |
| End | | 456 | 457 | 512 | 596 | 652 |
| Start AA | | 346 | 349 | 401 | 485 | 541 |
| Chain D | | ပ | ပ | ၁ | ວ | S |
| PDB ID | | lubd | 1ubd | 1ubd | Iubd | Iubd |
| SEQ B B S | | 485 | 485 | 485 | 485 | 485 |

| PDB annotation | COMPLEX (TRANSCREPTON REGILATIONDAN YING-YANG I; TRANSCREPTON INITIATION, INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRETION REGILATIONDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GI.J; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI, GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINIDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI, GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINIDNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | _ |
|-----------------|--|---|---|--|--|--|---|--|--|---|
| Coumpound | YYI; CHAIN: C, ADENO- SSOCIATED VRUS PS INITIATOR ELMENT DNA; CHAIN: A, B; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, |
| SeqFold | | | | | | 110.36 | | | | |
| PMF score | 0.98 | 60.0 | 0.47 | - | - | | -i | 0.88 | | 0.98 |
| Verify score | 0.06 | -0.05 | 0.01 | 0.4 | 0.53 | | 0.54 | 0.01 | -0.12 | 0.09 |
| PSI- BLAST | 3.40E-34 | 1.00E-26 | 5.60E-44 | 3.40E-31 | 1.40E-68 | 2.80E-77 | 2.80E-77 | 1.40E-73 | 1.10E-73 | 1.40E-72 |
| End | 089 | 262 | 346 | 343 | 402 | 458 | 458 | 542 | 654 | 681 |
| Start | 579 | 131 | | 207 | 263 | 319 | 319 | 375 | 487 | 516 |
| Chain | U | ¥ | V | A | ¥ | ¥ | Y | ¥ | 4 | ∢ |
| PDB ED | Jubd | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli |
| S e S | 485 | 485 | 485 | 485 | 485 | 485 | 485 | 485 | 485 | 485 |

| | | | | | | | | | | | | | | | | | | | | | | | | _ |
|-----------------|--|---|--|---|--|---|-----------------|-----------------------|--------------------|-------------------------|---------------------|---------------------|----------------------|-------------------|-------------------------|------------------------|-----------|---------------------|------------------|-----------------------|---------------------------|-----------|----------------------------|----------------------------|
| PDB annotation | ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINIDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | RNA BINDING PROTEIN G-PROTEIN, BETA-BARREL | RNA BINDING PROTEIN G-PROTEIN, BETA-BARREL | TRANSLATIONAL GTPASE EF-G RIBOSOMAL TRANSLOCASE, TRANSLATIONAL GTPASE | | | | | | TOWOT LEGOLD LEGOLD | M YOSIN MYOSIN MOTOR | | | | | MYOSIN MYOSIN MOTOR | | | | | MUSCLE PROTEIN MDE; MUSCLE | MUSCLE PROTEIN MDE; MUSCLE |
| Coumpound | D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ELONGATION FACTOR TU (EF-TU); CHAIN: A, B, C, D | ELONGATION FACTOR TU (EF-TU); CHAIN: A, B, C, D | ELONGATION FACTOR G; CHAIN: NULL; | ACYL-COENZYME A | BINDING PROTEIN ACYL- | COENZYME A BINDING | WITH LACA 3 PAI MITOYI. | COENZYME A (NMR, 20 | SIRUCTURES) IACA 4 | MIOSIN HEAVY CHAIN; | REGIL ATORY LIGHT | CHAIN; CHAIN: Y; MYOSIN | ESSENTIAL LIGHT CHAIN; | CHAIN: Z; | MYOSIN HEAVY CHAIN; | CHAIN: A; MYOSIN | CHAPL CITABLE WASCELN | COMMING CHAIN: 1; MITOSIN | CHAIN: 2: | MYOSIN; CHAIN: A, B, C, D, | MYOSIN; CHAIN: A, B, C, D, |
| SeqFold | | | | 627.43 | | | | | | | | 27,017 | 75.010 | | | | | | | | | | 524.14 | |
| PMF | | 96:0 | 0.95 | | - | 0.19 | 0.11 | | | | | | | | | | | _ | | | | | | |
| Verify score | | 0.23 | 0.03 | | 1.12 | -0.05 | -0.46 | | | | | | | | | | | 0.41 | | | | | | 0.58 |
| PSI- BLAST | | 1.40E-34 | 3.40E-33 | 0 | 0 | 3.40E-17 | 0.0014 | | | | | | > | | | | | 0 | | | | | 0 | 0 |
| End | | 159 | 619 | 454 | 454 | 192 | 1954 | | | | | 104 | ţ. | | | | | 807 | | | | | 765 | 769 |
| Start AA | | 523 | 251 | 28 | 28 | 49 | 1926 | | | | | | - | | | | | ^ | | | | | _ | 2 |
| Chain | | Ą | V | A | A | | | | | | | _ | | | | | 1 | ∢ | | | | | V | A |
| PDB DD | | 2gli | 2gli | 1d2e | 1d2e | 1dar | laca | | | | | 15.3 | 101 | | | | | 701 | | | | | Ibil | Ibr] |
| SEQ D NO: | | 485 | 485 | 486 | 486 | 486 | 487 | | | | | 107 | è | | | | | - 1 | | | | | 487 | 487 |

| | _ | | | | | | | | | | | | |
|------------------|-------------|-------------------------------------|-------------------------------------|---|--|--|---|---|---|--|--|--|---------------------------|
| PDB annotation | PROTEIN | MUSCLE PROTEIN MUSCLE PROTEIN | MUSCLE PROTEIN MUSCLE PROTEIN | TRANSFERASE BRUTONS AGAMAGGIOBULINEMA TYROSINE KINASE, BTK, TRANSFERASE, PH DOMAIN, BTK MOTIF, ZINC BINDING, X-LINKED 2 AGAMMAGIOBULINEMA, TYROSINE-PROTEN KINASE | SIGNAL TRANSDUCTION PROTEIN | SIGNAL TRANSDUCTION PROTEIN | TRANSMEMBRANE PROTEIN COLICIN, BACTERIOCIN, ION CHANNEL FORMATION, TRANSMEMBRANE 2 PROTEIN | TRANSMEMBRANE PROTEIN COLICIN, BACTERIOCIN, ION CHANNEL FORMATION, TRANSMEMBRANE 2 PROTEIN | STRUCTURAL PROTEIN TWO REPEATS OF SPECTRIN, ALPHA HELICAL LINKER REGION, 2.2 TANDEM 3-HELIX COLED-COILS, STRUCTURAL PROTEIN | STRUCTURAL PROTEIN TWO REPEATS OF SPECTRIN, ALPHA HELICAL LINKER REGION, 22 TANDEM 3-HELIX COLED-COILS, STRUCTURAL PROTEIN | CONTRACTILE PROTEIN MYOSIN MOTOR, CONFORMATIONAL CHANGES | MEMBRANE PROTEIN CRYSTAL STRUCTURE, MEMBRANE, FERM DOMAIN, TAIL DOMAIN | ENDOCYTOSIS/EXOCYTOSIS |
| Coumpound | E, F, G, H; | MYOSIN; CHAIN: A, B, C, D, E, F; | MYOSIN; CHAIN: A, B, C, D, E, F; | BRUTON'S TYROSINE KINASE, CHAIN: A, B; | BETA-SPECTRIN; IBTN 4 CHAIN: NULL; IBTN 5 | BETA-SPECTRIN; 1BTN 4 CHAIN: NULL; 1BTN 5 | COLICIN IA; CHAIN: NULL; | COLICIN IA; CHAIN: NULL; | ALPHA SPECTRIN; CHAIN: A, B, C, | ALPHA SPECTRIN; CHAIN: A, B, C; | MYOSIN HEAD; CHAIN: A; MYOSIN HEAD; CHAIN: Y; MYOSIN HEAD; CHAIN: Z; | MOESIN; CHAIN: A, B; MOESIN; CHAIN: C, D; | SYNTAXIN-1A; CHAIN: A. B, |
| SeqFold score | | | 470.06 | | | | | , | | | | | |
| PMF | | 1 | | 0.11 | 0.28 | 0.07 | -0.19 | -0.19 | -0.14 4 | -0.17 | _ | 66:0 | -0.2 |
| Verify score | | 95.0 | | -0.2 | 0.42 | -0.39 | 0.21 | 0.03 | 0.07 | 0.27 | 0.23 | 0.13 | 0.37 |
| PSI- BLAST | | 0 | 0 | 9.80E-08 | 8.40E-13 | 0.00042 | 2.80E-19 | 2.80E-18 | 1.40E-13 | 1.10E-14 | 0 | 4.20E-27 | 1.40E-11 |
| End | | 725 | 739 | 1495 | 1306 | 1382 | 933 | 61.6 | 940 | 946 | 807 | 2002 | 885 |
| Start AA | | = | = | 1394 | 1216 | 1318 | 796 | 810 | 726 | 808 | ~ | 1710 | 608 |
| Chain | | Ą | Ą | ¥ | | | | | V | ٧ | ∢ | ∢ | ٧ |
| PDB TD | | 1br2 | 1br2 | 類 | 1bh | 1btn | <u>'</u> B | <u>=</u> | lcun | lcun | ₩ ₩ | lefi Tel | lez3 |
| SEQ NO D | | 487 | 487 | 487 | 487 | 487 | 487 | 487 | 487 | 487 | 487 | 487 | 487 |

| PDB annotation | SYNAPTOTAGMIN ASSOCIATED 35 KDA PROTEIN, P35A, THREE HELIX BUNDLE | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGMIN ASSOCIATED 35 KDA PROTEIN, P35A, THREE HELIX BUNDLE | SIGNALING PROTEIN DAPPI, PHISH, BAMAZ; PLECKSTRIN, 3- PHOSPHONOSITIDES, INOSITOL. TETRAKUSPHOSPHATE 2 SIGNAL TRANSDUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN DAPPI, PHISH, BAMAZ; PLECKSTRIN, PHOSPHONOSITIDES, INOSITO, TETRAKUSPHOSPHATE 2 SIGNAL TRANSDUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN DAPPI, PHISH, BAMA3; BECKSTRIN, 3+ PHOSPHOINOSITIDES, INOSITOL TETRAKISPHOSPHATE 2 SIGNAL TRANSDUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN DAPPI, PHISH, BAMA3; HECKSTRIN, 3+ PHOSPHONOSITIDES, INOSITOL TETRAKISPHOSPHATE 2 SIGNAL TRANSDUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN DAPPI, PHISH, BAMAS, ELECKSRIN, PHOSPHONOSITIDES, INOSITOL TETRAKISPHOSPHATE 2 SIGNAL TEANSUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN DAPPI, PHISH, BAM32; PLECKSTRIN, 3- PHOSPHOINOSTIDES, INOSITOL TETRAKISPHOSPHATE 2 SIGNAL |
|------------------|---|---|--|--|---|--|--|--|
| Coumpound | Ú | SYNTAXIN-1A; CHAIN: A, B, C, | DUAL ADAPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | DUAL ADAPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | DUAL ADAFTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | DUAL ADAPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | DUAL ADAPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | DUAL ADAPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; |
| SeqFold score | | | | | | | | |
| PMF | | -0.18 | 0.92 | 0.96 | 0.36 | 66:0 | 0.86 | 0.25 |
| Verify score | | 0.3 | 0.43 | 0.13 | 0.19 | 0.54 | 90.0 | -0.03 |
| PSI- BLAST | | 1.10E-16 | 2.80E-22 | 7.00E-10 | 4.20E-10 | 5.60E-22 | 8.40E-10 | 1.40E-10 |
| End | | 933 | 1308 | 1382 | 1497 | 1308 | 1382 | 1497 |
| Start | | 814 | 1215 | 1331 | 1397 | 1215 | 1331 | 1397 |
| Chain ID | | 4 | <. | < | < | <` | ∢ | ¥ |
| PDB UD | | lez3 | 1fao | Ifao | Ifao | 1fb8 | 1108 | 1108 |
| SEQ B B SEQ | | 487 | 487 | 487 | 487 | 487 | 487 | 487 |

| PDB annotation | TRANSDUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN ARFI GUANINE NUCLEOTIDE EXCHANGE FACTOR AND PH DOMAIN | CELL ADHESION 3 SUBDOMAINS, CYTOSKELETON, CELL ADHESION | CONTRACTILE PROTEIN MYOSIN, DICTYOSTELIUM, MOTOR, MANT, ATPASE, ACTIN-BINDING, 2 COILED COIL | CONTRACTILE PROTEIN MYOSIN, DICTYOSTELIUM, MOTOR, MANT, ATPASE, ACTIN-BINDING, 2 COILED COIL | CONTRACTILE PROTEIN ATPASE, MYOSIN, COLIED COIL, ACTIN- BINDING, AFP-BINDING, 2 HEFYAD REPEAT PATTERN, METHYLATION, ARKYLATION, 3 PHOSPHORYLATION, CONTRACTILE PROTEIN. | CONTRACTILE PROTEIN ATPASE, MYOSIN, COLLED COLL, ACTIN. BINDING, AFF-BINDING, 2. HEFTAD REPEAT PATTERN, METHYLATION, A MKYLATION, 3 PHOSPHORYLATION, CONTRACTILE PROTEIN. | | |
|-------------------|---------------------------------------|---|---|--|--|---|---|---|--|
| Coumpound | | GRP1; CHAIN: A; | RADIXIN, CHAIN: A; | MYOSIN: CHAIN: NUEL; | MYOSIN, CHAIN: NULL; | MYOSIN; CHAIN: NULL; | MYOSIN; CHAIN: NULL; | PHOSPHORYLATION PLECKSTRIN (H-TEMINAL PLECKSTRIN HOMOLOGY DOMAIN) MUTANT IPLS 3 WITH LEU GLU (HIS)6 ADDED TO THE C TERMINUS IPLS 4 (INS(G105-LEHHRININ) NING, 25 STRUCTIPES) 19 S S | PHOSPHORYLATION PLECKSTRIN (N-TERMINAL PLECKSTRIN HOMOLOGY DOMAIN) MUTANT IPLS 3 |
| SeqFold score | | | | 540.6 | | 479.56 | | | |
| PMF | | 0.31 | - | | | | - | 0.46 | 0.04 |
| Verify score | | 0.21 | 0.08 | | . 9.0 | | 0.63 | 0.11 | -0.55 |
| PSI- BLAST | | 2.80E-16 | 2.80E-26 | 0 | 0 | 0 | 0 | 2.80E-17 | 5.60E-05 |
| End AA | | 1308 | 2044 | 739 | 222 | 671 | 119 | 1315 | 1381 |
| Start AA | | 1215 | 1710 | 7 | \$ | - | s | 1214 | 1342 |
| Chain ID | | ∢ | · | | | | | | |
| EDB CI | | Ifgy | 1gc7 | llvk | livk | lmn d | d d | lpls | lpls |
| SEQ BOS SOS | | 487 | 487 | 487 | 487 | 487 | 487 | 487 | 487 |

| | | | | | | | | | | , | |
|----------------|--|---|---|---|--|--|--|---|--|--|-----------------------|
| PDB annotation | | | SIGNAL TRANSDUCTION SON OF SEVENLESS; PLECKSTRIN, SON OF SEVENLESS, SIGNAL TRANSDUCTION | SIGNAL TRANSDUCTION SON OF SEVENLESS; PLECKSTRIN, SON OF SEVENLESS, SIGNAL TRANSDUCTION | SIGNAL TRANSDUCTION IRS-1; BETA-SANDWHICH, SIGNAL TRANSDUCTION | CONTRACTILE PROTEIN TRIPLE- HELIX COILED COIL, CONTRACTILE PROTEIN | MUSCLE PROTEIN, MYOSIN SUBFRAGMENT-1, MYOSIN HEAD, 2 MOTOR PROTEIN | MUSCLE PROTEIN MUSCLE PROTEIN, MYOSIN SUBFRAGMENT-1, MYOSIN HEAD, 2 MOTOR PROTEIN | MICROTUBULES MICROTUBULES, ALPHA-TUBULIN, BETA-TUBULIN, GTPASE HELIX | MICROTUBULES MICROTUBULES, ALPHA-TUBULIN, BETA-TUBULIN, GTPASE HELIX | KINASE KINASE, SIGNAL |
| Coumpound | WITH LEU GLU (HIS)6 ADDED TO THE C TERMINUS IPLS 4 (INS(G105- LEHHHHH)) (NMR, 25 STRUCTURES) IPLS 5 | PHOSPHORYA, ATTON PLECKSTRN (N-TEMINAL PLECKSTRN HOMOLOGY DOMAN) MUTANT 1PLS 3 WITH LEU GAU (HIS)6 ADDED TO THE C TERMINUS 1PLS 4 (INS(G165- LEHHHHBH) (NMK, 25 STRUCTURES) 1PLS 5 STRUCTURES) 1PLS 5 | SOS 1; CHAIN: NULL; | SOS I; CHAIN: NULL; | INSULIN RECEPTOR SUBSTRATE 1: CHAIN: A, B; | HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A; | MYOSIN; CHAIN: A, B, C; | MYOSIN; CHAIN: A, B, C; | TUBULIN; CHAIN: A, B; | TUBULIN; CHAIN: A, B; | CALCIUM/CALMODULIN- |
| SeqFold | | | | | | | 419.33 | | 727.18 | | |
| PMF score | | -0.01 | -0.01 | 0.05 | 0.25 | -0.13 | | _ | | _ | _ |
| Verify | | 0.02 | 10:0 | -0.14 | -0.27 | 0.05 | | 0.53 | | 8.0 | 0.35 |
| PSI- BLAST | | 9.80E-12 | 8.40E-15 | 0.00014 | 7.00E-07 | 1.30E-20 | 0 | 0 | 0 | 0 | 1.50E-87 |
| End | | 1495 | 1308 | 1381 | 1464 | 973 | 801 | 217 | 044 | 440 | 312 |
| Start | | 1394 | 1211 | 1331 | 1331 | T9T | 2 | 4 | _ | - | 91 |
| Chain ID | | | | | ¥ | ∢ | V | ٧ | ₹ | 4 | |
| PDB | | 1pls | Ipms | Ipms | lqqg | Iqui | 2mys | 2mys | dati | 1tub | 1a06 |
| SEQ No. | | 487 | 487 | 487 | 487 | 487 | 487 | 487 | 489 | 489 | 492 |

| PDB annotation | TRANSDUCTION, CALCIUM/CALMODULIN | KINASE KINASE, SIGNAL TRANSDUCTION, CALCILIM/CALMODIII.N | TRANSFERASE TRANSFERASE, SERINETHREONINE-PROTEIN KINASE, CASEIN KINASE, 2 SERTHR KINASE | | | PROTEIN KINASE CDK2; PROTEIN KINASE, CELL CYCLE, PHOSPHORYLATION, STAUROSPORINE, 2 CELL DIVISION, |
|------------------|---|---|--|--|--|--|
| Coumpound | DEPENDENT PROTEIN KINASE; CHAIN: NULL; | CALCIUM/CALMODULIN- DEPENDENT PROTEIN KINASE: CHAIN: NII I. | PROTEIN KINASE CKJ/ALPHA-SUBUNIT; CHAIN: NULL; | TRANSPERASPHORA ANGERASP CSAMPS- DEFENDENT PROTEIN KINASE (CLZ.1.1.3) (SCARSE) 1APM 3 (SCARSE) 1APM 3 ALPHA ISOBEZYME ALPHA ISOBEZYME ALPHA ISOBEZYME THE PETIDE 1APM 4 (S19AS) COMPLEX WITH THE PETIDE 1APM 4 (S19AS) COMPLEX WITH THE DETIBE 1APM 3 (S19AS) COMPLEX WITH | TRANSFERASE(PROSPHOTR ANSTERASE) SCAMPS- DEPRODENT PROTEIN SCRAFES) IAPM 3 GCATALYTOS UBUNIT) ALPHA ISOBENZYME ALTHA ISOBENZYME ALTHA ISOBENZYME THE PETTEINE IAPM 3 INBIDTOR RE(K)CAS AND ITHE DETTEINE IAPM STATE THE DETTEINE IAPM STATE THE DETTEINE IAPM STATE THE DETTEINE IAPM STATE STAT | CYCLIN-DEPENDENT PROTEIN KINASE 2; CHAIN: NULL; |
| SeqFold score | | 121.63 | 90.87 | | 158.35 | 120.73 |
| PMF | | | | - | | |
| Verify score | | | | 0.41 | - | |
| PS1- BLAST | | 1.50E-87 | 1.70E-43 | 0 | , | 1.00E-57 |
| End | | 318 | 316 | 315 | 333 | 314 |
| Start | | 17 | 2 | | m | 22 |
| Chain | | | | | ш | |
| PDB UD | | 1a06 | 1260 | da m | del m | laql |
| SE O O O | | 492 | 492 | 492 | 492 | 492 |

| PDB annotation | MITOSIS, INHIBITION | COMPLEX (KINASE/INHBITOR) CDK6, PI9INK4D; CYCLIN DEPENDENT KINASE, CYCLIN DEPENDENT KINASE, HIBITIORY 2 PROTEN, CDK, INK4, CELL, CYCLE, COMPLEX (KINASE/INHBITOR) | HEADUR HELM COMPLEX (INHIBITOR PROTEINKINSE) INHIBITOR RROTEIN CYCLIN-DEFENDENT KINASE, CELL CYCLEZ CONTROL, ALPHABETA, COMPLEX (INHIBITOR PROTEINKINASE) | TRANSFERASE CSK; PROTEIN KINASE, CTERMINAL SRC KINASE, PHOSPHORYLATION, 2 STAUROSPORINE, TRANSFERASE | PHOSPHOTRANSFERASE PROTEIN KINASE ICKI 18 | | | | |
|----------------|---------------------|---|---|---|--|---|---|---|---|
| Coumpound | | CYCLIN-DEPENDENT KINASE 6; CHAIN: A, C; CYCLIN-DEPENDENT KINASE INHIBITOR: CHAIN: B. D; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B; | C-TERMINAL SRC KINASE; CHAIN: A; | CASEIN KINASE I DELTA; ICKI 6 CHAIN: A, B; ICKI 7 | PHOSPHOTRANSFERASE CAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT ICMK 3 (E.C.2.7.1.37) ICMK 4 | PHOSPHOTRANSFERASE CAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT ICMK 3 (E.C.2.7.1.37) ICMK 4 | TRANSFERASE (PHOSPHOTR ANSFERASE) CAMP- DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (CAPK) ICTP 3 (CATALYTIC SUBUNIT) ICTP 4 | TRANSFERASE(PHOSPHOTR ANSFERASE) CAMP- DEPENDENT PROTEIN KINASE (E.C.Z.I.37) (CAPK) ICTP 3 (CATALYTIC |
| SeqFold | | 117.12 | 139.32 | 120.46 | . 6.28 | | 156.27 | | 152.26 |
| PMF | | | | | | _ | | _ | |
| Verify | | | | · | | 0.42 | | 0.32 | |
| PSI- BLAST | | 2.80E-54 | 1.40E-59 | 1.40E-39 | 9.80E-51 | 0 | 0 , | 0 | 0 |
| End | | 303 | 308 | 286 | 303 | 315 | 333 | 315 | 330 |
| Start | | 23 | 18 | 81 | 11 | _ | E | - | E . |
| Chain 19 | | ¥ | V | < | 4 | μl | ш | ш | ш |
| 808 En | T | 1bi8 | 16k | 1byg | lcki | k lcm | r la | lctp | lot db |
| SEQ NO DE | | 492 | 492 | 492 | 492 | 492 | 492 | 492 | 492 |

| PDB annotation | | TRANSFERASE KINASE DOMAIN, AUTOINHIBITORY FRAGMENT, HOMODIMER | TRANSFERASE KINASE DOMAIN, AUTOINHEBITORY FRAGMENT, HOMODIMER | PHOSPHOTRANSFERASE FORRIK, FIBROBLÁST GROWTH PACTOR RECEPTOR I; TRANSFERASE, TYGOSINE-BROTEIN KINASE, ATP. BINDING, 2 PHOSPHOTRANSFERASE RECEPTOR, PHOSPHOTRANSFERASE | PHOSPHOTAANSTERASE FGFR IK, FIBROBLAST GROWTH FACTOR RECEPTOR 1, TRANSTERASE, TYROSINE-RROTEIN KINASE, ATP. BINDING, 2 PHOSPHOTALTION, RECEPTOR, PHOSPHOTAANSFERASE | PROTEIN KÏNASE CDK2; TRANSFERASE, SERNETHREONINE PROTEIN KINASE, ATP-BINDING, 2 CELL CYCLE, CELL DIVISION, MITOSIS, PHOSPHORYLATION | SERINE/THREONINE-PROTEIN KINASE CSBP, RK, P38, PROTEIN SERTHR-KINASE, SERNE/THREONINE-PROTEIN KINASE | COMPLEX (TRANSFERASES/UBSTRATE) TYROSINE KTINASE, SIGNAL TRANSDUCTION, TRANSPORTORNASEPEQUE, 2 COMPLEX KINASEPETIDE SUBSTRATEATE |
|-----------------|-----------------|--|--|---|---|---|--|--|
| Coumpound | SUBUNIT) 1CTP 4 | SERINE/THREONINE- PROTEIN KINASE PAK- ALPHA; CHANI: A, B; SERINE/THREONINE- PROTEIN KINASE PAK- ALPHA; CHANI: C, D; | SERINETHREONINE- PROTEIN KINASE PAK- ALPHA; CHANI: A. B; SERINETHREONINE- PROTEIN KINASE PAK- ALPHA; CHANI: C. D; | FGF RECEPTOR 1; CHAIN: A, B; | FGF RECEPTOR 1; CHAIN: A, B; | HUMAN CYCLIN- DEPENDENT KINASE 2; CHAIN: NULL; | P38 MAP KINASE; CHAIN: NULL; | INSULIN RECEPTOR; CHAIN: A; PEPTIDE SUBSTRATE; CHAIN: B; |
| SeqFold | | | | 123.75 | 127.9 | 141.29 | 104.86 | 105.26 |
| PMF | | | - | | | | | |
| Verify score | | 0.38 | 0.21 | | | | | |
| PSI- BLAST | | 2.80E-69 | 5.10E-69 | 2.80E-38 | 1.20E-40 | 1.40E-60 | 2.80E-45 | 9.80E-40 |
| End AA | | 303 | 293 | 286 | 285 | 314 | 346 | 297 |
| Start | | ន | 4 | п | 12 | 8 | s | 6 |
| Chain ID | | ပ | υ | ٧ | | | | < |
| ED O | | 115m | 115m | 1億4 | <u>ğ</u> | Ibcl | lian | Ē |
| SEQ B B SE | | 492 | 492 | 492 | 492 | 492 | 492 | 492 |

| PDB annotation | ANALOG), ENZYME, 3 COMPLEX (TRANSFERASE/SUBSTRATE) | TRANSFERASE INK3; TRANSFERASE, INK3 MAP KINASE, SERINETHREONINE PROTEIN 2 KINASE | KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION | KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION | KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION | TRANSFERASE MITOGEN ACTIVATED PROTEIN KINASE, TRANSFERASE, MAP KINASE, EPENINTTUDEONIME PROTEIN | KINASE, 2 P38 | KINASE RABBIT MUSCLE PHOSPHORYLASE KINASE; | GLYCOGEN METABOLISM, | PROTEIN, 2 KINASE, ATP-BINDING, | KINASE RABBIT MUSCLE | PHOSPHORYLASE KINASE; | TRANSFERASE, SERINE/THREONINE- | PROTEIN, 2 KINASE, ATP-BINDING, CALMODULIN-BINDING | TRANSFERASE MAP KINASE, | SERINETHREONINE PROTEIN KINASE TRANSFERASE | SERINE KINASE SERINE KINASE. | TITIN, MUSCLE, AUTOINHIBITION | SERINE KINASE SERINE KINASE, | TRANSFERASE MITOGEN | ACTIVATED PROTEIN KINASE, MAP 2, | ERK2; TRANSFERASE, | SEKINE THREONINE-PROTEIN KINASE, MAP KINASE, 2 ERK2 |
|-----------------|--|---|--|--|--|---|---------------|---|----------------------|---------------------------------|------------------------|-----------------------|--------------------------------|---|-------------------------|--|------------------------------|-------------------------------|------------------------------|---------------------|----------------------------------|--------------------|--|
| Coumpound | | C-JUN N-TERMINAL KINASE; CHAIN: NULL; | TWITCHIN; CHAIN: NULL; | TWITCHIN; CHAIN: A, B; | TWITCHIN; CHAIN: A, B; | MAP KINASE P38; CHAIN: NULL; | | PHOSPHORYLASE KINASE; CHAIN: NULL; | | | PHOSPHORYL ASE KINASE: | CHAIN: NULL; | | | ERK2; CHAIN: NULL; | | TITIN; CHAIN: A. B. | | TITIN; CHAIN: A, B; | EXTRACELLIL AR | REGULATED KINASE 2; | CHAIN: NULL; | |
| SeqFold | | 127.36 | | 139.94 | | 121.52 | | 109.51 | | | | | | | 118.65 | | 126.69 | | | 130.2 | | | |
| PMF | | | _ | | 1 | | | | | | _ | | | | | | | | _ | | | | |
| Verify score | | | 0.27 | | 0.4 | | | | | | 9.0 | | | | | | | | 0.49 | | | | |
| PSI- BLAST | | 7.00E-54 | 1.70E-70 | 3.40E-71 | 3.40E-71 | 1.40E-56 | | 1.20E-81 | | | 1.20E-81 | | | | 5.60E-50 | | 4.20E-65 | | 4.20E-65 | 4.20E-56 | | | |
| End | | 357 | 334 | 321 | 284 | 350 | | 282 | | | 279 | | | | 341 | | 334 | | 274 | 346 | | | |
| Start | | | 22 | _ | 17 | 4 | | 22 | | | 23 | | | | 18 | | 61 | | 72 | = | | | |
| Chain D | | | | ¥ | 4 | | | | | | | | | | | | Ą | | ∢ | | | | |
| PDB CD | | 計 | Ikoa | 1kob | Ikob | 1p38 | | 1phk | | | 1phk | | | | 1pm | | 143 | | 譯 | 3erk | | | |
| SEQ No. us | | 492 | 492 | 492 | 492 | 492 | | 492 | | | 492 | | | • | 492 | | 492 | | 2 2 | 492 | | | |

| PDB annotation | LIPID TRANSPORT APO A-I; LIPOPROTEIN, LIPID TRANSPORT, CHOI ESTERDI METARDI ISM 2 | ATHEROSCLEROSIS, HDL, LCAT- ACTIVATION | TRANSFERASE IL-2-INDUCIBLE T- CELL KINASE; TRANSFERASE, REGULATORY INTRAMOLECULAR COMPLEX, KINASE | COMPLEX (ADAPTOR PROTEINFETTIED) ASH, GROWTH PACTOR RECEPTOR-BOUND PROTEIN 2; COMPLEX (ADAPTOR PROTEIN/PEPTIDE), SISI DOMAIN, 2 GUANINE-NUCLEOTIDE RELEASING FACTOR. | COMPLEX (TRANSFERASEPEPTIDE) COMPLEX (TRANSFERASEPEPTIDE), SIGNAL TRANSDUCTION, 2 SH3 DOMAIN | | | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGMIN ASSOCIATED 35 KDA PROTEIN, P35A, THREE HELIX BUNDLE | MEMBRANE PROTEIN FOUR HELIX BUNDLE, ALPHA HELIX | TRANSFERASE PROTO-ONCOGENE TYROSINE KINASE; PROTO- ONCOGENE, TRANSFERASE, |
|-----------------|---|--|--|--|--|--|--|---|--|---|
| Coumpound | APOLIPOPROTEIN A-1; CHAIN: A, B, C. D; | | ITK; CHAIN: NULL; | GRB2; CHAIN: A; SOS; CHAIN: B; | ABL TYROSINE KINASE; CHAIN: A, C, B, G; PEPTIDE P41; CHAIN: B, D, F, H; | PROTEIN/PETIDE) C-CRK (N-TERAINAL SH3 DOMAN) (CCKRSH3-N) WITH ICKA 3 CG PETIDE (PRO-PRO-PRO-PRO-PRO-PRO-PRO-PRO-PRO-PRO- | PHOSPHOTRANSFERASE C- SRC KINASE (SH3 DOMAIN) (E.C.2.7.1.112) ICSK 3 | SYNTAXIN-1A; CHAIN: A, B, C, | SSOI PROTEIN; CHAIN: A; | PHOSPHOTRANSFERASE FYN; CHAIN: A; 3BP-2; CHAIN: B; |
| SeqFold | 66.14 | | | | | | | | | |
| PMF score | | | 0.75 | - | 0.95 | 0.99 | 66.0 | 0.05 | 0.05 | 0.88 |
| Verify score | | | 0.64 | 0.47 | 0.67 | 0.58 | 0.72 | 0.22 | 0.24 | 0.02 |
| PSI- BLAST | 0.0042 | | 1.70E-08 | 4.20E-19 | 7.00E-18 | 8.40E-18 | 9.80E-19 | 2.80E-06 | 0.0056 | 2.80E-17 |
| End | 278 | | 440 | 445 | 444 | . 442 | 442 | 214 | 256 | 444 |
| Start AA | 58 | | 370 | 388 | 390 | 389 | 387 | 83 | 166 | 385 |
| Chain ID | A | | | ⋖ | ¥ | ∢ | ∢ | V . | ¥ | ¥ |
| PDB CD | laví | | lawj | laze | 1bbz | lcka | lcsk | 1cz3 | 1fio | 1fyn |
| Se Si | 493 | | 493 | 493 | 493 | 493 | 493 | 493 | 493 | 493 |

| | | | | | | | | | _ | |
|------------------|---|--|--|---|---|--|--|---|-----|---|
| PDB annotation | TYROSINE-PROTEIN KINASE, 2 PHOSPHORYLATION, ATP-BINDING, MYRUSTYLATION, SH3 DOMAIN, 3 COMPLEX (PHOSPHOTRANSFERASEPEPTIDE) | COMPLEX (SIGNAL TRANSDUCTION/PEPTIDE) COMPLEX (SIGNAL TRANSDUCTION/PEPTIDE), SH3 DOMAIN | | SIGNAL TRANSDUCTION ADAPTOR SH2, SH3 1GR 14 | | TYROSINE-PROTEIN KINASE BRUTONS TYROSINE KINASE, B CELL PROCENITOR KINASE, TRANSFERASE, TYROSINE-PROTEIN KINASE, PHOSPHORYLATION, 2 SH3 DOMAIN | PROTEIN TRANSPORT HELIX-TURN- HELIX TPR-LIKE REPEAT, PROTEIN TRANSPORT | TRANSFERASE HCK; SH3, PROTEIN TYROSINE KINASE, SIGNAL TRANSDUCTION, 2 TRANSFERASE | | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC |
| Coumpound | | GRB2; CHAIN: A; SOS-1; CHAIN: B; | SIGNAL TRANSDUCTION PROFIEM SHOWTH PACTOR RECEPTOR-BOUND PROTEIN 3 SH3 DOMANN COMPLEXED WITH SOSA PETIDE IGRA 4 (NMR, 29 STRUCTURES) IGRS, 2 | GROWTH FACTOR BOUND PROTEIN 2; IGRI 5 CHAIN: A, B: IGRI 6 | PHOSPHORIC DIESTER HYDROLASE PHOSPHOLIPASE C-GAMMA (SH3 DOMAIN) (E.C.3.1.4.11) HSQ 3 (NMK, MINIMIZED MEAN STRUCTURE) 1180 4 | TYROSINE-PROTEIN KINASE BTK; CHAIN: A; | VESICULAR TRANSPORT PROTEIN SEC17; CHAIN: A; | HEMATOPOIETIC CELL KINASE; CHAIN: NULL; | | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX |
| SeqFold score | | | | | | , | 69.94 | | | 82.45 |
| PMF | | _ | _ | 0.43 | 0.99 | 0.98 | | 0.99 | | |
| Verify | | 0.34 | 0.47 | 0.34 | 9.0 | 0.47 | | 0.1 | | |
| PSI- BLAST | | 2.80E-18 | 5.60E-19 | 1.10E-16 | 2.80E-18 | 4.20E-18 | 4.20E-07 | 7.00E-19 | | 5.60E-35 |
| End AA | | 442 | 444 | 444 | 444 | 444 | 262 | 444 | 1 | 422 |
| Start AA | | 388 | 380 | 272 | 383 | 389 | _ | 385 | 9,6 | 342 |
| Chain D | | < | ∢ . | V | | ¥ | A | | Į. | < |
| PDB ID | | lgbq | lgbr | Igri | Ihsq | 1qly | Iqqe | 4hck | | lalh |
| SEQ No: | | 493 | 493 | 493 | | 493 | 493 | 493 | 9 | 458 |

| PDB annotation | FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERODNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGENDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC |
|------------------|---|---|--|--|---|---|---|---|--|--------------------------------|
| Coumpound | OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN: CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; |
| SeqFold score | | | | | | | | 110.98 | | |
| PMF | | _ | 0.77 | - | _ | - | | | | 0.87 |
| Verify score | | 0.03 | 0.12 | 0.38 | 9.4 | 0.24 | 0.34 | | 0.05 | -0.05 |
| PSI- BLAST | | 5.60E-35 | 1.40E-33 | 6.80E-49 | 1.70E-50 | 3.40E-51 | 5.10E-51 | 3.40E-51 | 3.40E.47 | 4.20E-36 |
| End AA | | 478 | 303 | 338 | 366 | 394 | 422 | 423 | 477 | 202 |
| Start | | 370 | 398 | 257 | 285 | 313 | 341 | 341 | 397 | 397 |
| Chain | | ٧ | Y | ပ | ပ | v | O | ပ | ပ | ၁ |
| E CE | | ialh | laih | Jme y | Jme y | y y | y y | y y | y me | Ime |
| S a S | | 498 | 498 | 498 | 498 | 498 | 498 | 498 | 498 | 498 |

| PDB annotation | FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC : FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION) REGULATION/DNA), RNA POLYMERASER II, 2 TRANSCRIPTION INITIATION, ZNO FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASER II, 2 TRANSCRIPTION NITIATION, 2NAC PROBER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION) REGULATION/DNA), RNA REGULATION/DNA), RNA POLYMERASE BIL, 2 TRANSCRIPTION INITIATION, ZNO FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA |
|------------------|---|--|--|--|--|--|---|--|
| Coumpound | CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA, CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | TFIIIA: CHAIN: A, D: 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F, | TFIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F, | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F. | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; |
| SeqFold score | | | | | | 102.44 | | · |
| PMF | | | - | -0.15 | -0.01 | | 0.94 | 0.92 |
| Verify score | | 0.23 | 0.19 | 0.1 | 90.00 | | 0.11 | -0.02 |
| PSI- BLAST | | 1.00E-49 | 1.70E-35 | 3.40E-12 | 1.00E-33 | 1.40E-68 | 1.70E-36 | 8.50E-39 |
| End AA | | 505 | 511 | 282 | 375 | 447 | 437 | 487 |
| Start | | 424 | 452 | 255 | 221 | 285 | | 342 |
| Chain | | ပ | ပ | 5 | ∢ | ∢ | ¥ | A |
| PDB CI | > | y y | lme y | lme y | 1168 | 1466 | 148 | 146 |
| S e S | | 498 | 498 | 498 | 498 | 498 | 498 | 498 |

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|------------------|---|---|--|---|---|---|--|
| PDB annotation | POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONIDNA) COMPLEX (TRANSCRIPTION REGULATIONIDNA), RNA REGULATIONIDNA), RNA POLYMERASE III, 2 TRANSCRIPTION NATTA ATON 7 7000 FINCER PROTEN | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-YANO I; TRANSCRIPTION INITIATION MITIATIOR RELABENT YYI, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULATIONINA YING-YAND !; TRANSCRIPTON INITIATION INITIATIOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REQUILATIONINA) YING-YANG I; TRANSCRIPTON INITIATION, INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REQUILATIONDA), TMG-YAND I; TRANSCRIPTION INITIATION, TRANSCRIPTION INITIATION, TRANSCRIPTION INITIATION, TRANSCRIPTION, 20MPLEX RECOGNITION, 3 COMPLEX TRANSCRIPTION REGULATIONDA), | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN |
| Coumpound | | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DINA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DINA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITATOR ELEMENT DNA; CHAIN: A, B; |
| SeqFold score | | | | | 88.23 | | |
| PMF | | 0.95 | 0.05 | - | | - | - |
| Verify score | | 0.14 | -0.02 | 0.25 | , | 0.23 | 0.36 |
| PSI- BLAST | | 8.50E:35 | I.00E-30 | 1.70E-34 | 2.80E-56 | 2.80E-56 | 8.50E-35 |
| End | | 507 | 338 | 366 | 395 | 394 | 394 |
| Start AA | | 370 | 228 | 265 | 285 | 290 | 293 |
| Chain | | ∢ | U | O | o | U | ပ |
| 80 E | | <u>9</u> | lubd | lubd | Pqn | Inbd | lubd |
| S a S | | 498 | 498 | 498 | | 498 | 498 |

| | | | | | | | | | | | | | _ | | | | | | | | | | | |
|------------------|---|--|--------------------------------|--|---|--|---|---------------------------|--|----------------------|---------------------------|---------------------------|----------------------|---------------------------|------------------------------------|--|---------------------------|--|---------------------------|------------------------------------|----------------------|---|----------------------------|---------------------------|
| · PDB annotation | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DIA) YING-YANG 1; TRANSCRIPTION INITIATION | INITIATOR ELEMENT, YY1, ZINC 2 | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX PRANSCEPPTION DEGLII ATTOMONAY | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | ZINC FINGER COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTFIN/DNA) FIVE-FINGER GLT: GLT | ZINC FINGER, COMPLEX (DNA- | 1-1 |
| Coumpound | | YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATIOR ELEMENT DIVA: | CHAIN: A, B; | | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; CHAIN: A, B; | | ZINC FINGER PROTEIN GLI1; | CHAIN: A; DNA; CHAIN: C, D; | | ZINC FINGER PROTEIN GLII; | CHAIN: A; DINA; CHAIN: C, | î | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, | ä | ZINC FINGER PROTEIN GUII; | CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, | ň | ZINC FINGER PROTEIN GLII; | Ď. | ZINC FINGER PROTEIN GLII; |
| SeqFold score | | | | | | | | | | | 81.78 | | | | | | | | | | | | | |
| PMF | | _ | | | 0.92 | | | 0.28 | | | | | | _ | | | | | 98.0 | | | 0.41 | | 0.48 |
| Verify score | | 0 | | | -0.07 | | | -0.26 | | | | | | 0.24 | | | 0.36 | | 0.14 | | | 0.17 | | 0.04 |
| PSI- BLAST | | 2.80E-56 | | | 6.80E-36 | | | 8.50E-33 | | | 2.80E-70 | | | 2.80E-70 | | | 3.40E-33 | | I.30E-63 | | | 4.20E-61 | | 6.80E-32 |
| End AA | | 422 | | | 202 | | | 337 | | | 423 | | | 422 | | | 423 | | 479 | | | 202 | | 504 |
| Start AA | | 311 | | | 405 | | | 200 | | | 285 | | | 290 | | | 293 | | 313 | | | 341 | | 377 |
| Chain El Gi | | ၁ | | | U | | | ¥ | | | ٧ | | | Ą | | | Y | | V | | | Ą | | V |
| 10B | | Pqn1 | | | Inpq | | | 2gli | | | 2gli | | | 2gli | | | 2gli | | 2gli | | | 2gli | | 2gli |
| S e S | | 498 | | | 498 | | | 498 | | | 498 | | | 498 | | | 498 | | 498 | | | 498 | | 498 |

| PDB annotation | PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | LIGASE CYCLIN A/CDK2- ASSOCIATED PROTEIN P45, CYCLIN A/CDK2-ASSOCIATED PROTEIN P19, SKP1, SKP2, F-BOX, LRK, LEUCINE- RICH REPEAT, SCF, UBIQUITIN, 2 E3, UBIOUTIN PROTEIN LGASE | LIGASE SKP2 F-BOX; SKP1, SKP1, SKP2, SKP2, SKP2, F-BOX, LRR, LEUCINE-RICH REPEAT, SCF, UBIQUITIN, 2 E3, UBIQUITIN PROTEIN LIGASE | LIGASE CBL, UBGHT, ZAP-70, E2, UBQUITIN, E3, PHOSPHORYLATION, 2 TYROSINE KINASE, UBQUITINATION, PROTEIN DEGRADATION, | TRANSCRIPTION REGULATION PROTO-ONCOGENE, NUCLEAR BODIES (PODS), LEUKEMIA, 2 TRANSCRIPTION REGULATION | | | LIGASE CBL, UBCH7, ZAP-70, E2, UBRQUITIN, E3, PROSPRORYLATION, 2 TYROSINE KINASE, UBRQUITINATION, PROTEIN DEGRADATION, |
|----------------|--|--|--|---|---|---|---|--|
| Coumpound | CHAIN: A; DNA; CHAIN: C, D; | SKP; CHAIN: A, C, E, G, I, K, M, O; SKP1; CHAIN: B, D, F, H, J, L, N, P; | CYCLIN A/CDK2- ASSOCIATED P19; CHAIN: A, C; CYCLIN A/CDK2- ASSOCIATED P45; CHAIN: B, D; | SIGNAL TRANSDUCTION PROTEIN CBI; CHAIN: A; ZAP-10 PEPTIDE; CHAIN: B; UBIQUITIN-CONJUGATING ENZYME E12-18 KDA UBCH7; CHAIN: C; | TRANSCRIPTION FACTOR PML; CHAIN: NULL; | VIRUS EQUINE HERPES VIRUS-1 (C3HC4, OR RING DOMAIN) ICHC 3 (NMR, 1 STRUCTURE) ICHC 4 | VIRUS EQUINE HERPES VIRUS-1 (C3HC4, OR RING DOMAIN) ICHC 3 (NMR, 1 STRUCTURE) ICHC 4 | SIGNAL TRANSDUCTION - PROTEIN CBL, CHAIN: A; ZAP-70 PETTIDE, CHAIN: B; UBIQUITIN-CONUGATING ENZYME E12-18 KDA UBCH7; CHAIN: C; |
| SeqFold | | | | | | | | |
| PMF | | 0.52 | 0.53 | 0.16 | 0.01 | 0.53 | 69:0 | 0.81 |
| Verify | | -0.78 | -0.81 | 0.08 | -0.37 | -0.07 | 0.02 | -0.55 |
| PSI- BLAST | | 0.0007 | 2.80E-06 | 1.70E-06 | 1.40E-13 | 8.40E-17 | 3.40E-16 | 5.60E-11 |
| End | | 57 | 57 | 907 | 305 | 323 | 316 | 307 |
| Start | | | 28 | 998 | 255 | 259 | 261 | 262 |
| Chain | | A | ٧ | ∢ | | | | < |
| 8 <u>8</u> a | | . Ift | 131 | Ifbv | Ibor | 1chc | lchc | Ifbv |
| S e S | | 499 | 499 | 200 | 201 | 501 · 1chc | 201 | 501 |

| PDB annotation | LIGASE CBL, UBCH7, ZAP-70, E2, UBIQUITIN, B2, PHOSPHORYLATION, 21 TYSOSINE KUNASE, UBIQUITINATION, PROTEIN DEGRADATION, | METAL BINDING PROTEIN RING FINGER PROTEIN MAT1; RING FINGER (C3HC4) | DAA-BINDING PROTEIN V(D) RECOMBINATION ACTUVATING PROTEIN I: ACII, V(D) RECOMBINATION, ANTIBODY, MAD, RING FINDER, 2 ZINC BINUCLEAR CLUSTER, ZINC FINGER, DIAA- | DA-BINDING PROTEIN V(DJ) RECOMBINATION ACTIVATING PROTEIN I: ACII, V(DJ) RECOMBINATION, ANTIBODY, MAD, RING PROER, Z ZINC BINCCLEAR CLUSTER, ZINC FINGER, DNA- BINDING PROTEIN | MEMBRANE PROTEIN LECTIN-LIKE, NEUROBIOLOGY, CELL-CELL ADHESION, CELL-CELL 2 RECOGNITION, ALTERNATIVE SPLICING, MEMBRANE PROTEIN | TRANSFERASE DINUCLEOTIDE- BINDING MOTIF, PHOSPHORIBOSYL TRANSFERASE | TRANSFERASE DINUCLEOTIDE- BINDING MOTE, PHOSPHORIBOSYL TRANSFERASE | TRANSFERASE DINUCLEOTIDE- BINDING MOTIF, PHOSPHORIBOSYL TRANSFERASE | ZINC METALLOPROTEASE P. AERUGINOSA ALKALINE PROTEASE; IKAP 6 CALCIUM BINDING PROTEIN |
|------------------|---|---|--|--|---|---|--|---|--|
| Coumpound | SIGNAL TRANSDUCTION PROTEIN CBI, CHAIN: A; ZAP-70 PEPTIDE, CHAIN: B; UBIQUITIN-CONUGATING ENZYME E12-18 KDA UBCH7; CHAIN: C; | CDK-ACTIVATING KINASE ASSEMBLY FACTOR MAT1; CHAIN: A; | RAGI; CHAIN: NULL; | RAGI; CHAIN: NULL; | NEUREXIN-1 BETA; CHAIN: A, B, C, D, E, F, G, H; | NICOTINATE MONONUCLEOTIDE:5,6- CHAIN: A; | NICOTINATE MONONUCLEOTIDE:5,6- CHAIN: A; | NICOTINATE MONONUCLEOTIDE:5,6- CHAIN: A; | ALKALINE PROTEASE; IKAP 4 CHAIN: P; IKAP 5 TETRAPEPTIDE (GLY SER |
| SeqFold score | | | | | | | | | |
| PMF | - | 0.22 | 0.94 | 0.45 | -0.11 | -0.2 | -0.18 | -0.2 | -0.2 |
| Verify score | -0.24 | -0.17 | -0.11 | -0.27 | 0.21 | 0.3 | 0.51 | 0.56 | 96'0 |
| PSI- BLAST | 1.70E-09 | 7.00E-13 | 8.40E-18 | 1.70E-09 | 1.40E-17 | 1.10E-23 | 1.30E-20 | 1.10E-23 | 1439 7.00E-14 |
| End AA | 310 | 319 | 333 | 342 | 224 | 1380 | 22.01 | 1241 | 1439 |
| Start | 263 | 259 | 239 | 263 | 20 | 1042 | 753 | 116 | 1076 |
| Chain | ∢ | ¥ | | | ¥ | A | Ψ. | ٧ | Ь |
| PDB ID | 1fbv | 1825 | Ітид | Пт | 1c4r | sop1 | s0P1 | 1d0s | lkap |
| SEQ B) B) | 501 | 105 | 501 | 501 | 202 | 505 | 205 | 205 | 205 |

| PDB annotation | IKAP 19 | ZINC METALLOPROTEASE P. AERUGINOSA ALKALINE PROTEASE; IKAP 6 CALCIUM BINDING PROTEIN IKAP 19 | ZINC METALLOPROTEASE P. AERUGINOSA ALKALINE PROTEASE; IKAP 6 CALCIUM BINDING PROTEIN IKAP 19 | ZINC METALLOPROTEASE P. AERUGINOSA ALKALINE PROTEASE; IKAP 6 CALCIUM BINDING PROTEIN IKAP 19 | OUTER MEMBRANE PROTEIN OSMOPORIN; OUTER MEMBRANE PROTEIN, NON-SPECIFIC PORIN, OSMOPORIN, 2 BETA-BARREI, TRANSMEMBRANE | OUTER MEMBRANE PROTEIN OSMOPORIN; OUTER MEMBRANE PROTEIN, NON-SPECIFIC PORIN, OSMOPORIN, 2 BETA-BARREI, TRANSNEMBRANE | OUTER MEMBRANE PROTEIN OSMOPORIN; OUTER MEMBRANE PROTEIN, NON-SPECIFIC PORIN, OSMOPORIN, 2 BETA-BARREI, TRANSKEMBRANE | | | METAL BINDING PROTEIN BETA SANDWICH, CALCIUM-BINDING PROTEIN, METAL BINDING 2 |
|------------------|---------------------------------------|---|---|---|---|---|---|---|---|---|
| Coumpound | ASN SER); 1KAP 9 CHAIN: I; 1KAP 10 | ALKALINE PROTEASE; IKAP 4 CHAIN: P; IKAP 5 IETRAPEPTIDE (GLY SER ASN SER); IKAP 9 CHAIN: I; IKAP 10 | ALKALINE PROTEASE; IKAP 4 CHAIN: P; IKAP 5 TETRAPEPTIDE (GLY SER ASN SER); IKAP 9 CHAIN: I; IKAP 10 | ALKALINE PROTEASE; IKAP 4 CHAIN: P; IKAP 5 TETRAPEPTIDE (GLY SER ASN SER); IKAP 9 CHAIN: I; IKAP 10 | OMPK36; CHAIN: A, B, C; | OMPK36; CHAIN: A, B, C; | OMPK36, CHAIN: A, B, C; | OUTER MEMBRANE PROTEIN PHOSPHOPORIN (PHOE) IPHO 3 | OUTER MEMBRANE PROTEIN PHOSPHOPORIN (PHOE) 1PHO 3 | LAMININ ALPHA2 CHAIN; CHAIN: A, B, C, D; |
| SeqFold score | | | | | | | | | | |
| PMF | | -0.19 | -0.2 | -0.19 | -0.2 | -0.19 | 0.2 | -0.2 | -0.19 | 0.1 |
| Verify score | | 3 | 1.03 | 0.87 | 1.07 | 1.04 | 0.87 | 0.83 | 1.15 | 0.51 |
| PSI- BLAST | | 5.60E-10 | 8.40E-14 | 1.10E-13 | 1.10E-31 | 1.40E-32 | 4.20E-27 | 1.40E-23 | 7.00E-27 | 2.80E-13 |
| End | | 743 | 858 | 1244 | 1348 | 1043 | 1241 | 1045 | 1214 | 225 |
| Start | | 482 | 530 | 068 | 1004 | 707 | 875 | 692 | 872 | 78 |
| Chain TO | | a, . | ۵, | ρ. | < | ∢ | Y | | | 4 |
| PDB ID | | Ikap | lkap | Ikap | losm | losm | losm | 1pho | Ipho | lqu0 |
| SEQ NO: | | 502 | 202 | 502 | 502 | 202 | 502 | 502 | 502 | 202 |

| | _ | | | | | | | | | | | |
|-----------------|---------|---|--|--|--|--|--|--|--|--|---|---|
| PDB annotation | PROTEIN | INTEGRAL MEMBRANE PROTEIN PORIN MATRIX PORIN, OMPF PORIN; 20MF 7 PORIN, MEMBRANE PROTEIN 20MF 12 | TRANSFERASE PROTEIN-ACETYL COENZYME A COMPLEX, ACETYLTRANSFERASE | SIGNAL TRANSDUCTION PROTEIN | SIGNAL TRANSDUCTION PROTEIN | CYTOSKELETON | CYTOSKELETON | CYTOSKELETON | SIGNALING PROTEIN DAPPI, PHISH, BAM22; PECKSTRIN, 3-PHOSPHOINOSITIDES, INOSITOL TETRAKISPHOSPHATE 2 SIGNAL TRANSDUCTION PROTEIN, ADAPTOR | rotein | SIGNAL TRANSDUCTION SON OF SEVENLESS; PLECKSTRIN, SON OF SEVENLESS, SIGNAL TRANSDUCTION | ACTIN-BINDING PROTEIN ACTIN- BINDING PROTEIN, CALCIUM- |
| Coumpound | | MATRIX PORIN OUTER MEMBRANE PROTEIN F; 20MF 5 CHAIN: NULL; 20MF 6 | HPA2 HISTONE ACETYL TRANSFERASE; CHAIN: A, B, C, D; | BETA-SPECTRIN; 1BTN 4 CHAIN: NULL; 1BTN 5 | BETA-SPECTRIN; IBTN 4 CHAIN: NULL; IBTN 5 | BETA-SPECTRIN; IDRO 6 CHAIN: NULL: IDRO 7 | BETA-SPECTRIN; IDRO 6 CHAIN: NULL: IDRO 7 | BETA-SPECTRIN; IDRO 6 CHAIN: NULL; IDRO 7 | DUAL ADAPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | PHOSPHORYLATION PLECKSTRIN (A-TERMALL PLECKSTRIN (H-SWAMALL DOMAN) MUTART IPLS 3 WITH LEU GLU (HIS)6 ADDED TO THE C TEMMINGS IPLS 4 (INS(GIOS- LEHHERMAN) (NAR, 25 STRUITTIRES) IPLS 5 KTRUITTIRES) IPLS 6 | SOS 1; CHAIN: NULL; | T-FIMBRIN; CHAIN: NULL; |
| SeqFold | | | | | | 50.76 | | | | | | |
| PMF | | -0.18 | 90.0 | 98.0 | 0.78 | | 0.39 | 0.75 | -0.07 | 0.16 | 0.01 | 0.72 |
| Verify score | | 1 | -0.12 | 0.36 | 0.38 | | 80.0 | 0.35 | 0.15 | 0.05 | -0.02 | -0.05 |
| PSI- BLAST | | 7.00E-21 | 0.0028 | 1.70E-22 | 2.80E-24 | 7.00E-28 | 5.10E-17 | 7.00E-28 | 3.40E-17 | 1.70E-18 | 2.80E-14 | 1.20E-32 |
| End AA | | 1202 | 282 | . 181 | 187 | 192 | 130 | 681 | 185 | 188 | 190 | 250 |
| Start | | 842 | . 122 | 82 | 83 | 73 | 83 | 35 | 88 | 88 | 80 | 107 |
| Chain ID | | | ٧ | | | | | | ∢ | | | |
| PDB CD | | 2omf | 1qsm | 1btn | 1btn | 1dro | Idro | Idro | Ifao | lpls | Ipms | laoa |
| SeQ No. ID | | 202 | 909 | 207 | 202 | 202 | 507 | 507 | 507 | 507 | 507 | 208 |

| PDB annotation | BINDING, PHOSPHORYLATION | STRUCTÚRAL PROTEIN DYSTROPHIN, MUSCULAR DYSTROPHY, CALPONIN HOMOLOGY DOMAIN, 2 ACTIN-BINDING, UTROPHIN | STRUCTURAL PROTEIN CALPONIN HOMOLOGY DOMAIN, DOMAIN SWAPPING, ACTIN BINDING, 2 UTROPHIN, DYSTROPHIN, STRUCTURAL PROTEIN | STRUCTURAL PROTEIN TWO REPEATS OF SPECTRIN, ALPHA HELICAL LINKER REGON, 2.2 TANDEM 3-HELIX COLED-COLLS, STRUCTURAL PROTEIN | ENDOCYTOSIS/EXOCYTOSIS NSEC1; | MULTI-SUBUNIT | ENDOCYTOSIS/EXOCYTOSIS NSECI; PROTEIN-PROTEIN COMPLEX, MILLT-SLIBILINIT | ENDOCYTOSIS/EXOCYTOSIS NSECI- | PROTEIN-PROTEIN COMPLEX, MULTI-SUBUNIT | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGMIN ASSOCIATED 35 KDA PROTEIN, P35A, THREE HELIX BINDLE | MEMBRANE PROTEIN FOUR HELIX BUNDLE, ALPHA HELIX | CONTRACTILE PROTEIN TRIPLE- | PROTEIN | CHAPERONE HSP40; CHAPERONE, HEAT SHOCK, PROTEIN FOLDING, DNAK | CHAPERONE HSP40; CHAPERONE, HEAT SHOCK, PROTEIN FOLDING, |
|----------------|--------------------------|--|---|--|-------------------------------|------------------------|---|-------------------------------|--|--|--|--|---------|---|---|
| Coumpound | | DYSTROPHIN; CHAIN: A, B, C, D; | UTROPHIN ACTIN BINDING REGION; CHAIN: A, B; | ALPHA SPECTRIN; CHAIN: A, B, C; | SYNTAXIN BINDING | SYNTAXIN IA; CHAIN: A; | SYNTAXIN BINDING PROTEIN I; CHAIN: A; SYNTAXIN IA: CHAIN: B: | SYNTAX IN BINDING | PROTEIN I; CHAIN: A; SYNTAXIN IA; CHAIN: B; | SYNTAXIN-1A; CHAIN: A, B, C, | SSO1 PROTEIN; CHAIN: A; | HUMAN SKELETAL MUSCLE AI PHA.ACTININ ? CHAIN: | A; | DNAJ; CHAIN: NULL; | DNAJ; CHAIN: NULL; |
| SeqFold | | | | | | | | | | | | | | 71.72 | |
| PMF | | 0.03 | 0.27 | 60.0 | 0.05 | | 0.3 | 0.03 | | 0.03 | 0.18 | 90.0 | | | 1 |
| Verify | | -0.01 | 10:0 | 90:0- | -0.13 | | -0.31 | -03 | | 0.25 | -0.45 | -0.12 | | | 0.45 |
| PSI- BLAST | | 8.50E-30 | 1.70E-29 | 2.80E-09 | 1.40E-18 | | 1.10E-10 | 1.10E-08 | | 1.10E-09 | 2.80E-05 | 4.20E-21 | | 6.80E-33 | 6.80E-33 |
| End | | 248 | 248 | 562 | 460 | | 195 | 940 | | 933 | 686 | 467 | | 124 | 122 |
| Start | | 106 | 110 | 365 | 208 | | 364 | 713 | | 804 | 794 | 205 | | 94 | 47 |
| Chain ID | | ٧ | Α . | ¥ | В | | e e | В | | ∢ ; | V | ٧ | | | |
| PDB CD | | ldxx | lqag | Icun | IdhI | | Idal | Idal | | 23 | OJ I | Idun | | 1bq0 | 1bq0 |
| SEQ NO: | | 508 | 508 | 515 | 515 | | 515 | 515 | | 515 | 515 | 515 | | 516 | 516 |

| | | | | _ | | _ | | | | | | | _ | | | | | | _ | | | | | | | | |
|------------------|------|---|---|---|---|---------------------|----------|-----------------------|--------------------|---------------------|----------------------------|--|----------------|--|-----------|-------------|----------------------|-----------------------------|--------------|-------------------|------------------------|------------------|--------------------|----------------------|------------------|--------------------|--------------------------------------|
| PDB annotation | DNAK | MOLECULAR CHAPERONE HDJ-1; MOLECULAR CHAPERONE | MOLECULAR CHAPERONE HDJ-1; MOLECULAR CHAPERONE | | | | | | | | SUGAR BINDING PROTEIN BETA | TREFOIL, MULTILECTIN RECEPTOR, PITUITARY HORMONES, 2 SULFATED CARBOHYDRATE | TD ANGEGD A CE | GLYCOSYLTRANSFERASE | | TRANSFERASE | GEI COSTEIRAISEERASE | HYDROLASE XYLAN DEGRADATION | | | | | | | | | |
| Coumpound | | HUMAN HSP40; CHAIN: NULL; | HUMAN HSP40; CHAIN: NULL; | | COMPLEX (GLYCOSIDASE/CARBOHYD RATE) ABRIN-A COMPLEXED WITH TWO | SUGAR CHAINS 1ABR 3 | COMPLEX | (GLYCOSIDASE/CARBOHYD | COMPLEXED WITH TWO | SUGAR CHAINS 1ABR 3 | MANNOSE RECEPTOR; | CHAIN: A; | SPORE COAT | POLYSACCHARIDE BIOSYNTHESIS PROTEIN | CHAIN: A; | SPORE COAT | BIOSYNTHESIS PROTEIN | ENDO-1,4-BETA-XYLANASE; | CHAIN: A, B; | GLYCOSIDASE RICIN | (E.C.3.2.2.2.2) 2001 3 | OXYGEN TRANSPORT | HEMOGLOBIN (DEOXY, | HUMAN FETAL F=/IIS=) | OXYGEN TRANSPORT | HEMOGLOBIN (DEOXY, | HUMAN FEIAL F=/II3=) IFDHG I IFDHH 2 |
| SeqFold score | | 52.89 | | | | | | | | | | | | | | | | | | | | 112.26 | | | | | |
| PMF | - | | - | | 0.01 | | 0.04 | | | | 0.13 | | = | | | 0 | | 96.0 | | 50:0 | | | | | _ | | |
| Verify score | | | 0.21 | | -0.08 | | 0.04 | | | | -0.22 | | 71.0 | | | -0.1 | | 90.0 | į |) (1.0 | | | | | 0.29 | | |
| PSI- BLAST | | 1.00E-30 | 1.00E-30 | | 1.40E-10 | | 6.80E-30 | | | | 0.0017 | | 5.10E-23 | | | 7.00E-45 | | 1.70E-31 | 1 700 00 | 1. /UE-28 | | 1.00E-39 | | | 1.00E-39 | | |
| End AA | į | 125 | 122 | | 547 | | 547 | | | | 213 | | 333 | | | 371 | | 548 | 473 | È | I | 32 | | | 92 | | |
| Start AA | ļ | 46 | 48 | | 378 | | 412 | | | | 444 | | Ξ | | | Ξ | | 422 | 413 | | | _ | | | _ | | |
| Chain D | | | | | ф | | æ | | | | ∢ | | | | | ∢. | | ¥ | - | α . | | G | | | O | | |
| PDB ID | - | l lud | 1hđj | | labr . | | labr | | | | 1998 | | logo | i | | lqgq | | lxyf | :000 | 1007 | T | 15 | | | 1£ | | |
| Se Se | ì | 910 | 516 | | 522 | | 225 | | | 985 | 775 | | 522 | | | 225 | | 522 | \$33 | 776 | | 523 | | | 523 | | |

| PDB annotation | OXYGEN STORAGE/TRANSPORT HEMOGLOBIN, DEOXY FORM | TRANSFERASE IL-2-INDUCIBLE T. CELL KINASE; TRANSFERASE, REGULATORY INTRAMOLECULAR COMPLEX, KINASE | COMPLEX (ADAPTOR PROTEINFETHED) ASH, GROWTH PACTOR RECEPTOR-BOUND PROTEIN 2: COMPLEX (ADAPTOR PROTEIN/PETHED), SH5 DOMAIN, 2 GUANINE-AUGLEOTIDE RELEASING FACTOR | MYOSIN MYOSIN MOTOR | MYOSIN MYOSIN MOTOR | MUSCLE PROTEIN MDE; MUSCLE PROTEIN | MUSCLE PROTEIN MDE, MUSCLE PROTEIN | MUSCLE PROTEIN MUSCLE PROTEIN | MUSCLE PROTEIN MUSCLE PROTEIN | CONTRACTILE PROTEIN MYOSIN MOTOR, CONFORMATIONAL CHANGES | |
|------------------|--|--|--|--|---|---|--|-------------------------------------|-------------------------------------|--|--|
| Coumpound | HEMOGLOBIN; CHAIN: A, C; HEMOGLOBIN; CHAIN: B, D; | ITK; CHAIN; NULL; | GRB2, CHAIN: A; SOS; CHAIN: B: | MYOSIN HEAVY CHAIN; CHAIN: A; MYOSIN REGULATORY LIGHT CHAIN; CHAIN: Y; MYOSIN ESSENTAL LIGHT CHAIN; CHAIN: Z. | MYOSIN HEAVY CHAIN; CHAIN: A; MYOSIN REGULATORY LIGHT CHAIN; CHAIN: Y; MYOSIN ESSENTIAL LIGHT CHAIN; CHAIN: Z. | MYOSIN; CHAIN: A, B, C, D, E, F, G, H; | MYOSIN; CHAIN: A, B, C, D, E, F, G, H; | MYOSIN; CHAIN: A, B, C, D, E, F; | MYOSIN; CHAIN: A, B, C, D, E, F; | MYOSIN HEAD; CHAIN: A; MYOSIN HEAD; CHAIN: Y; MYOSIN HEAD; CHAIN: Z; | SIGNAL TRANSDUCTION PROTEIN GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2 (GRB2, N-TERMINAL IGBR |
| SeqFold score | | | | 335.35 | | | 352.11 | 339.22 | | | |
| PMF | - | 0.15 | 0.89 | | - | - | | | - | | 0.72 |
| Verify | 90:0 | 0.45 | 0.5 | | 0.34 | 0.59 | | | 0.44 | 0.01 | 0.45 |
| PSI- BLAST | 7.00E-40 | 1.40E-18 | 2.80E-18 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1.10E-19 |
| End | 32 | 1088 | 1087 | 739 | 739 | 708 | 711 | 629 | 619 | 739 | 1089 |
| Start | - | 1018 | 1037 | - . | * | - | | - | _ | _ | 1028 |
| Chain | В | | • | < | ∢ | 4 | ٧ | ٧ | ٧ | ٧ | ۷ |
| EQB CD | lgcv | lawj | laze | 1671 | 1671 | lbr1 | 둳 | 1br2 | 1br2 | ī∯ | 1gbr |
| S e S | 523 | 526 | 526 | 526 | 526 | 526 | 526 | 226 | 226 | 326 | 526 |

| PDB annotation | | | SIGNAL TRANSDUCTION ADAPTOR SH2, SH3 IGRI 14 | | CONTRACTILE PROTEIN MYOSIN, DICTYOSTELIUM, MOTOR, MANT, ATPASE, ACTIN-BINDING, 2 COILED COIL | CONTRACTILE PROTEIN MYOSIN, DICTYOSTELIUM, MOTOR, MANT, ATPASE, ACTIN-BINDING, 2 COILED COIL | CONTRACTILE PROTEIN ATPASE, MYOSIN, COLIED COLI, ACTIN. BINDING, ATP-BINDING, 2 HEPTAD REPEAT PATTERN, METHYLATION, ARKYLATION, PROTEIN N. PROTEIN CONTRACTILE PROTEIN | CONTRACTILE PROTEIN ATPASE, MYOSIN, COLIED COLI, ACTIN. BINDING, ATP-BINDING, 2 HEPTAD REPEAT ATTERN, METHYLATION, A ALKYLATION, 3 PHOSPHORYLATION, CONTRACTILE PROTEIN |
|-----------------|--|--|---|---|--|--|--|---|
| Coumpound | 3 SH3 DOMAIN) COMPLEXED WITH SOS-A PEPTIDE IGBR 4 (NMR, 29 STRUCTURES) IGBR 5 | ADAFTOR PROTEIN CONTAINING SH2 AND SH3 GROWTH FACTOR RECEPTOR-BOUND PROTEIN 2 (GRB2) IGFC 3 (C- PERMIANL, SH3 DOMAIN) (NMR, MINIMIZED MEAN STRUCTURD IGFC 4 STRUCTURD IGFC 4 | GROWTH FACTOR BOUND PROTEIN 2; IGRI 5 CHAIN: A, B; IGRI 6 | PHOSPHORIC DIESTER HYDROLASE PHOSPHOLIPASE C-GAMMA (SH3 DOMAIN) (E.C.3.1.4.11) HSQ 3 (NMR, MINIMIZED MGAN STRUCTURE) 1HSQ 4 | MYOSIN; CHAIN: NULL; | MYOSIN; CHAIN: NULL; | MYOSIN; CHAIN: NULL; | MYOSIN; CHAIN: NULL; |
| SeqFold | | | | | | 348.12 | 269.23 | |
| PMF score | | 0.59 | 0.12 | 1202.08 | 1 | | | |
| Verify score | | 0.29 | -0.23 | 0.24 | 0.18 | | <u></u> | 0.37 |
| PSI- BLAST | | 1.30E-19 | 8.40E-17 | 1.40E-18 | 0 | 0 | 0 | 0 |
| End AA | | 6801 | 1089 | 1089 | 879 | 619 | 809 | 809 |
| Start AA | | 1035 | 896 | 1032 | ı | _ | _ | - |
| Chain D | | | ¥ | | | | | |
| PDB CD | | 1gfc | lgri | lhsq | Ilvk | livk | Jmn d | lmn d |
| Se Se | | 526 | 526 | 526 | 226 | 526 | 526 | 226 |

| PDB annotation | CIRCULAR PERMUTANT PWT; CIRCULAR PERMUTANT, SH3 DOMAIN, CYTOSKELETON | TYROSINE-PROTEIN KINASE BRUTONS TYROSINE KINASE, B CELL PROCENITOK KINASE, TRANSFERASE, TYROSINE-PROTEIN KINASE, PHOSPHORYLATION, 2 SH DÖMAIN | SIGNAL TRANSDUCTION PROTEIN SICHOMOLOGY 3 (SH3) DOMAIN, PEPTIDE-BINDING PROTEIN, ISEM 18 2 GUANINE NUCLEOTIDE EXCHANGE FACTOR ISEM 19 | MUSCLE PROTEIN MUSCLE PROTEIN, MYOSIN SUBFRAGMENT-1, MYOSIN HEAD, 2 MOTOR PROTEIN | MUSCLE PROTEIN MUSCLE PROTEIN, MYOSIN SUBFRAGMENT-1, MYOSIN HEAD, 2 MOTOR PROTEIN | TRANSFERASE HCK; SH3, PROTEIN TYROSINE KINASE, SIGNAL TRANSDUCTION, 2 TRANSFERASE | ELECTRON TRANSPORT ELECTRON TRANSPORT, THIOL-DISULFIDE OXDOREDUCTASE, 2 THIOLTRANSFERASE, THIOREDOXIN SUPERFAMILY | ELECTRON TRANSPORT ELECTRON TRANSPORT, THIOL-DISULFIDE OXIDOREDUCTASE, 2 THIOLTRANSFERASE, THIOREDOXIN SUPERFAMILY | TRANSFERASE ACETYLTRANSFERASE | TRANSFERASE AAC; AMINOGLYCOSIDE 6-N- ACETYLTRANSFERASE, ANTIBIOTIC |
|-----------------|--|---|---|---|---|---|---|--|---|--|
| Coumpound | ALPHA SPECTRIN; CHAIN: NULL; | TYROSINE-PROTEIN KINASE BTK; CHAIN: A; | SEM-5; ISEM 3 CHAIN: A, B; ISEM 5 10-RESIDUE PROLINE-RICH PEPTIDE FROM MSOS ISEM 8 CHAIN: C, D ISEM 10 | MYOSIN; CHAIN: A, B, C; | MYOSIN; CHAIN: A, B, C; | HEMATOPOIETIC CELL KINASE; CHAIN: NULL; | GLUTAREDOXIN 3; CHAIN: NULL; | GLUTAREDOXIN 3; CHAIN: NULL; | ARYLALKYLAMINE N- ACETYLTRANSFERASE; CHAIN: A, B; | AMINOGLYCOSIDE NG- ACETYLTRANSFERASE TYPE 1; CHAIN: A; |
| SeqFold | | | | | 267.23 | | | | | |
| PMF | -1.41 | -1.41 | 0.94 | _ | | 0.18 | 0.68 | 0.96 | 96.0 | 0.95 |
| Verify score | 29.0 | 0.25 | 0.63 | -0.02 | | 0.32 | -0.21 | 0.17 | 0.25 | 0.29 |
| PSI- BLAST | 7.00E-20 | 4.20E-18 | 4.20E-19 | 0 | 0 | 1.10E-18 | 0.0015 | 9.80E-06 | 3.40E-19 | 6.80E-08 |
| End | 6801 | 1089 | 6801 | 731 | 737 | 1089 | 96 | 68 | 159 | 184 |
| Start | 1032 | 1036 | 1035 | - | _ | 1032 | 41 | 23 | 41 | 24 |
| Chain | | ∢ | ∢ | ∢ | 4 | | | | æ | < |
| e a | lpwt | 1qb | lsem | Zmys | 2mys | 4hck | Звих | Звл | 1991 | 1687 |
| S B S | 526 | 226 | 526 | 526 | 526 | 526 | 528 | 528 | 529 | 529 |

| PDB annotation | 2 RESISTANCE, ACETYL COENZYME A | TRANSFERASE N-ACETYL TRANSFERASE | SIGNALING PROTEIN P300/CBP ASSOCIATED FACTOR, COENZYME A, ACETYL/TRANSFERASE, 2 COACTIVATOR, SIGNALING PROTEIN | SIGNALING PROTEIN P300/CBP ASSOCIATED FACTOR, COENZYME A, ACETYLTRANSFERASE, 2 COACTIVATOR, SIGNALING PROTEIN | TRANSFERASE PROTEIN-ACETYL COENZYME A COMPLEX, ACETYLTRANSFERASE | TRANSFERASE PROTEIN-ACETYL COENZYME A COMPLEX, ACETYLTRANSFERASE | TRANSFERASE HISTONE ACETYLTRANSFERASE, GCNS- RELATED N-ACETYLTRANSFERASE, 2 COA BINDING PROTEIN | GENE REGULATION ADAG; TRANSCRIPTIONAL REGULATION, HISTONE ACETYLATION, N. P. ACETYLTRANSFERASE, GCNS RELATED NA ACETYLTRANSFERASE FAMILY, 3 GENE REGULATION | CONTRACTILE PROTEIN TROPOMYOSIN COLLED-COIL ALPHA- HFI ICAL CONTRACTI E PROTEIN | CONTRACTILE PROTEIN TROPOMYOSIN COLLED-COLL ALPHA-HELICAL, CONTRACTILE PROTEIN | CONTRACTILE PROTEIN TROPOMYOSIN COILED-COIL ALPHA- HELICAL, CONTRACTILE PROTEIN | CONTRACTILE PROTEIN |
|------------------|------------------------------------|--|--|--|--|--|---|---|---|--|---|------------------------|
| Coumpound | | SEROTONIN N- ACETYL TRANSFERASE; CHAIN: A; | P300/CBP ASSOCIATING FACTOR; CHAIN: B, A; | P300/CBP ASSOCIATING FACTOR; CHAIN: B, A; | HPA2 HISTONE ACETYLTRANSFERASE; CHAIN: A, B, C, D; | HPA2 HISTONE ACETYL TRANSFERASE; CHAIN: A, B, C, D; | TGCNS HISTONE ACETYL TRANSFERASE; CHAIN: A; | TRANSCRIPTIONAL ACTIVATOR GCNS; CHAIN: A, B; | TROPOMYOSIN; CHAIN: A, B, C, D | TROPOMYOSIN; CHAIN: A, B, C, D | TROPOMYOSIN; CHAIN: A, B, C, D | TROPOMYOSIN; CHAIN: A, |
| SeqFold | | | | | | - | | | | | | |
| PMF | | 0.88 | 0.81 | 61.0 | 0.33 | 0.23 | 0.19 | 0.04 | _ | 0.64 | 0.94 | |
| Verify score | | 0.5 | 0.39 | 0.15 | 0.13 | 0.15 | -0.06 | 60.0 | -0.48 | -0.17 | -0.17 | -0.48 |
| PSI- BLAST | | 1.20E-19 | 2.80E-13 | 1.70E-05 | 1.50E-13 | 4.20E-19 | 3.40E-07 | 1.00E-05 | 1.50E-54 | 3.40E-49 | 5.10E-53 | 1.50E-54 |
| End | | 159 | 174 | 184 | 156 | 165 | 183 | 179 | 296 | 245 | 248 | 296 |
| Start AA | | 14 | 36 | 77 | = | 12 | 79 | 08 | 3 | E. | E | 3 |
| Chain 10 | | ٧ | æ. | ф | V | ¥ | ٧ | | A | 4 | ٧ | V |
| PDB DD | | lcjw | m o | e o | lqsm | lqsm | lqst | lygh | lclg | lclg | lelg | Iclg |
| SEQ ID NO: | | 529 | 529 | 529 | 529 | 529 | 529 | 529 | 534 | 534 | 534 | 535 |

| PDB annotation | TROPOMYOSIN COILED-COIL ALPHA- HELICAL, CONTRACTILE PROTEIN | CONTRACTILE PROTEIN TROPOMYOSIN COILED-COIL ALPHA- HELICAL, CONTRACTILE PROTEIN | CONTRACTILE PROTEIN TROPOMYOSIN COILED-COIL ALPHA-HELICAL, CONTRACTILE PROTEIN | COMPLEX (INHIBITOR/NUCLEASE) COMPLEX (INHIBITOR/NUCLEASE), COMPLEX (IRAND, HYDROLASE 2 MOLECULAR RECOGNITION, REPROPEMAPPING, LEUCINE-RICH 3 REPEATS | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP, RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP, RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP, RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP, RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP, RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP, RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP, RIBONUCLEOPROTEIN | CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL ADHESION | CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL |
|------------------|--|---|--|--|--|--|--|--|--|--|--|---|---|
| Coumpound | B, C, D | TROPOMYOSIN; CHAIN: A, B, C, D | TROPOMYOSIN; CHAIN: A, B, C, D | RIBONUCLEASE INHIBITOR; CHAIN: A, D; ANGIOGENIN; CHAIN: B, E; | UZ RNA HAIRPIN IV; CHAIN: Q, R; UZ A'; CHAIN: A, C; UZ B"; CHAIN: B, D; | U2 RNA HARPIN IV; CHAIN: Q, R; U2 A; CHAIN: A, C; U2 B"; CHAIN: B, D; | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | INTERNALIN B; CHAIN: A; | INTERNALIN B; CHAIN: A; |
| SeqFold score | | | | | | | | | | | | | |
| PMF | | 0.64 | 0.94 | 0.47 | | 0.45 | 0.29 | 0.12 | 6.0 | 0.29 | 0.03 | 0.8 | 0.21 |
| Verify | | -0.17 | -0.17 | 0.29 | 0.75 | 0.42 | 0.59 | -0.09 | 0.65 | 0.48 | 0.1 | 0.41 | 0.19 |
| PSI- BLAST | | 3.40E-49 | 5.10E-53 | 4.20E-25 | 2.80E-22 | 4.20E-18 | 0.00017 | 3.40E-06 | 5.60E-23 | 0.00017 | 3.40E-06 | 1.70E-22 | 1.00E-16 |
| End | | 245 | 248 | 306 | 297 | 306 | 284 | 144 | 301 | 284 | 144 | 286 | 350 |
| Start | | 3 | 3 | 9 | 136 | 164 | 210 | 40 | 136 | 210 | 40 | 127 | 183 |
| Chain | | ¥ | Ψ. | 4 | ¥ | 4 | ¥ | 4 | ၁ | ပ | U | ¥ | V |
| FDB ED | | lclg | lclg | la4y | 1a9n | la9n | 1a9n | 1a9n | 1a9n | la9n | 1a9n | 1406 | 1406 |
| S a S | | 535 | 535 | 538 | 538 | 238 | 538 | 538 | 538 | 538 | 538 | 538 | 538 |

| PDB annotation | | CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL ADHESION | CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL ADHESION | CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL ADHESION | TRANSFERASE CRYSTAL STRUCTURE, RAB | GEKANYLGEKANYLIKANSFEKASE, | FORMYLMETHIONINE, ALPHA | SUBUNII, BEIA SUBUNII | CONTRACTILE PROTEIN LEUCINE- | RICH REPEAT, BETA-BETA-ALPHA | CTUINDER, DYNEIN, Z CHLAMYDOMONAS, FLAGELLA | RNA BINDING PROTEIN TAP (NFXI); | RIBONUCLEOPROTEIN (RNP, RBD OR | RRM) AND LEUCINE-RICH-REPEAT 2 (LRR) | RNA BINDING PROTEIN TAP (NFXI); | EOPROTEIN (RNP, RBD OR | RRM) AND LEUCINE-RICH-REPEAT 2 (LRR) | RNA BINDING PROTEIN TAP (NFX1); | KIBONUCLEOPKO LEIN (KNP,KBD UK | DECOMPENDED FOR EAT 2 | LIGASE CYCLIN A/CDK2- | A/CDK2-ASSOCIATED PROTEIN P19: | SKP1, SKP2, F-BOX, LRR, LEUCINE- | RICH REPEAT, SCF, UBIQUITIN, 2 E3, UBIQUITIN PROTEIN LIGASE | LIGASE CYCLIN A/CDK2- ASSOCIATED PROTEIN P45; CYCLIN |
|------------------|----------|---|---|---|---------------------------------------|----------------------------|-------------------------|-----------------------|------------------------------|------------------------------|--|---------------------------------|--------------------------------|---|---------------------------------|------------------------|--------------------------------------|---------------------------------|--------------------------------|-----------------------|--------------------------------|--------------------------------|----------------------------------|---|--|
| | ADHESION | CELL ADHE REPEAT, CA ADHESION | CELL ADHE REPEAT, CA ADHESION | CELL ADHE REPEAT, CA ADHESION | TRANSFERASE CR STRUCTURE, RAB | 2 0 A 2 RESC | FORMYLME | SUBUNIT, B | CONTRACT | RICH REPE/ | CHLAMYDO | RNA BINDIP | RIBONUCLE | RRM) AND I | RNA BINDIR | REGONDELE | (LRR) AND I | RNA BINDIN | PPM AND | (LRR) | LIGASE CYC | A/CDK2-ASS | SKP1, SKP2, | RICH REPEA | LIGASE CYC ASSOCIATE |
| Coumpound | | INTERNALIN B; CHAIN: A; | INTERNALIN B; CHAIN: A; | INTERNALIN B; CHAIN: A; | RAB GERANYLGERANYLTRANSF | CHAIN A C. RAB | GERANYLGERANYLTRANSF | CHAIN: B. D. | OUTER ARM DYNEIN; | CHAIN: A; | | NUCLEAR RNA EXPORT | FACTOR 1; CHAIN: A, B; | | NUCLEAR RNA EXPORT | FACTOR 1; CHAIN: A, B; | | NUCLEAR RNA EXPORT | FACTOR I; CHAIN: A, B; | | SKP2; CHAIN: A, C, E, G, I, K, | H.J.L.N.P. | | | SKP2; CHAIN: A, C, E, G, I, K, M, O; SKPI; CHAIN: B, D, F, |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.11 | 0.15 | 0.22 | -0.14 | | | | 91.0 | | | 0.13 | | | 0.03 | | | 0.1 | | | 0.49 | | | | -0.09 |
| Verify score | | 0.3 | 0.05 | 0.17 | 0.02 | | | | -0.03 | | | -0.32 | | | -0.1 | | | -0.4[| | | 0.63 | | | | 0.08 |
| PSI- BLAST | | 5.10E-24 | 1.00E-25 | 8.50E-25 | 1.20E-09 | | | | 6.80E-13 | | | 1.00E-06 | | | 1.70E-07 | | | 1.00E-06 | | | 5.10E-13 | | | | 2.80E-17 |
| End | | 162 | 161 | 212 | 130 | | | | 143 | | | 120 | | | 290 | | | 120 | | ٠ | 284 | | | | 339 |
| Start AA | | E . | 32 | 27 | 7 | | | | 91 | | | . 52 | | | 227 | - | | 22 | | | 111 | | | | 6 |
| Chain D | | V | ¥ | · • | ٧ | | | | V | | | V | | | В | | | e e | | | ¥ | | | | 4 |
| EQ CO | | 140b | 90P1 | 1d0b | Idce | | | | 6sp1 | | | 161 | _ | | 161 | | | 1601 | | | ıtğı | | | | lfqv |
| S e S | | 538 | 538 | 538 | 238 | | | | 538 | | | 538 | _ | | 238 | | | 238 | | | 538 | | | | 238 |

| PDB annotation | A/CDK2-ASSOCIATED PROTEIN P19, SKP1, SKP2, F-BOX, LRR, LEUCINE- RICH REPEAT, SCF, UBIQUITIN, 2 E3, UBIQUITIN PROTEIN LIGASE | LIGASE CYCLIN A/CDK2- ASSOCIATED P45, CYCLIN A/CDK2- ASSOCIATED P19, SKP1, SKP2, F-BOX, LRRS, LEUCINE-RICH REPEATS, SCF, 2 UBIQUITIN, E3, UBIQUITIN PROTEIN LIGASE | LIGASE CYCLIN A/CDK2- ASSOCIATED P45, CYCLIN A/CDK2- ASSOCIATED P19, SKP1, SKP2, F-BOX, LRRS, LEUGNE-RICH REPEATS, SCF, 2 UBRQUITIN, E3, UBRQUITIN PROTEIN LIGASE | TRANSCRIPTON RAAIP, RANGAP, GITASE-ACTIVATING PROTEIN POR SPII, GTPASE-ACTIVATING RROTEIN, GAP, RAAIP, RANGAP, LRR, LEUCINE-2 RICH REPEAT PROTEIN, TWINNING, JARGHEBRAL TWINNING, JARGHEBRAL | ACETYLATION RNASE INHIBITOR, RIBONUCLEASE/ANGIOGENIN INHIBITOR ACETYLATION, LEUCINE- RICH REPEATS | LIGASE TRPRS; CLASS I TRNA SYNTHETASE, AARS, INDUCED FIT, TRPRS | SIGNALING PROTEIN OXYGEN SENSOR, HISTIDINE KINASE, PAS, HIGH-RESOLUTION, TWO- 2 COMPONENT SYSTEM | IRON STORAGE IRON STORAGE, MULTIGENE FAMILY, ACETYLATION | IRON STORAGE IRON STORAGE, |
|-----------------|--|---|---|--|--|---|---|---|----------------------------|
| Coumpound | H, J, L, N, P; | SKP2; CHAIN: A, C, SKP1; CHAIN: B, D; | SKP2; CHAIN: A, C, SKP1; CHAIN: B, D; | GTPASB-ACTIVATING PROTEIN RNAI_SCHPO; CHAIN: A. B. | RIBONUCLEASE INHIBITOR; CHAIN: NULL; | TRYPTOPHANYL TRNA SYNTHETASE: CHAIN: A, B, C, D, E, F; | NITROGEN FIXATION REGULATORY PROTEIN FIXL; CHAIN: A; | FERRITIN; CHAIN: NULL; | FERRITIN; CHAIN: NULL; |
| SeqFold | | | | | | | | 194.39 | |
| PMF | | 0.24 | 0 | -0.11 | 0.22 | _ | 0.23 | | - |
| Verify score | | 0.13 | 0.29 | 0.26 | 0.43 | 95.0 | 0.23 | | 0.36 |
| PSI- ·BLAST | | 5.10E-13 | 1.30E-23 | 2.80E-22 | 1.40E-32 | 0 | 4.20E-17 | 7.00E-84 | 7.00E-84 |
| End | | 284 | 306 | | 311 | 359 | 371 | 199 | 138 |
| Start AA | , | Ш | 84 | 98 | 69 | 35 | 274 | 30 | 30 |
| Chain ID | | ¥ | ¥ | ¥ | | A | Α . | | |
| PDB CD | | 1162 | 162 | lyrg | 2bnh | 1d2r | 1406 | lacw | laew |
| SEQ B B S | | 538 | 538 | 238 | 238 | 539 | 540 | 541 | 541 |

| PDB annotation | MULTIGENE FAMILY, ACETYLATION | IRON STORAGE IRON STORAGE, DIIRON | IRON STORAGE IRON STORAGE, DIIRON | IRON STORAGE IRON STORAGE | IRON STORAGE IRON STORAGE | IRON STORAGE IRON STORAGE | ISOMERASE ISOMERASE, PPIASE | COMPLEX (ISOMERASE/PEPTIDE) | COMPLEX (ISOMERASEPEPTIDE), CYCLOPHILIN A, HIV-1 CAPSID, 2 BEETING SYSTAGETTY | FSEUDO-SIMMEINI | COMPLEX (ISOMERASEPEPTIDE) COMPLEX (ISOMERASEPEPTIDE), CYCLOPHILIN A, HIV-1 CAPSID, 2 PSEUDO-SYNMETRY | | | COMPLEX | (ISOMERASE/IMMUNOSUPPRESSANT) | CYCLOSPORIN, ISOMERASE, | KOLAMASE, SIGNAL ICTIN 19 | COMPLEX | (ISOMERASE/IMMUNOSUPPRESSANT) | CYCLOSPORIN, ISOMERASE, ROTAMASE, SIGNAL ICYN 19 | | ISOMERASE(PEPTIDYL-PROLYL CIS- TRANS) PEPTIDYL-PROLYL CIS- |
|-----------------|-------------------------------|--|---|---------------------------|---------------------------|---------------------------|------------------------------|-----------------------------|---|--|---|--|---|-----------------------|-------------------------------|-------------------------|---------------------------|-----------------------|-------------------------------|---|-------------------|---|
| Coumpound | | M FERRITIN; CHAIN: A,B,C,D,E,F,G,H,IJ,K,L,M,N,O P,O,R,S,T,U,V,W,X; | M FERRITIN; CHAIN: A,B,C,D,E,F,G,H,I,J,K,L,M,N,O P,O,R,S,T,U,V,W,X; | FERRITIN; CHAIN: NULL; | FERRITIN; CHAIN: NULL; | FERRITIN; CHAIN: NULL; | CYCLOPHILIN; CHAIN: NULL; | CYCLOPHILIN A; CHAIN: A; | PEPTIDE FROM THE HIV-1 CAPSID PROTEIN; CHAIN: B; | The same of the sa | CYCLOPHILIN A; CHAIN: A; PEPTIDE FROM THE HIV-1 CAPSID PROTEIN; CHAIN: B; | ISOMERASE(PEPTIDYL- PROLYL CIS-TRANS) CYCLOPHILIN (NMR, 12 STRUCTURES) ICLH 3 | ISOMERASE(PEPTIDYL- PROLYL CIS-TRANS) CYCLOPHILIN (NMR, 12 STRICTI IBES) ICI H 3 | CYCLOPHILIN B: ICYN 6 | CHAIN: A; 1CYN 7 [D- | (CHOLINYL)ALA]8- | CHAIN: C; 1CYN 11 | CYCLOPHILIN B; ICYN 6 | CHAIN: A; 1CYN 7 [D- | CYCLOSPORIN; 1CYN 10 | CHAIN: C; ICYN 11 | CYCLOPHILIN 3; CHAIN: A; |
| SeqFold | | 221.42 | | 284.09 | | | 94.49 | 89.5 | | | | 9.69 | | 103.11 | | | | | | | | |
| PMF | | | _ | | 1 | - | | | | | _ | | 0.46 | | | | | _ | | | | 1 |
| Verify score | | | 0.53 | | 0.5 | 0.5 | | | | į | 0.7 | | 0.28 | | | | | 0.52 | | | | 0.62 |
| PSI- BLAST | | 5.60E-88 | 5.60E-88 | 1.40E-75 | 1.40E-75 | 1.00E-74 | 5.10E-29 | 5.10E-38 | | 00 000 | 5.10E-38 | 8.40E-39 | 8.40E-39 | 5.10E-34 | | | | 5.10E-34 | | | | 1.70E-34 |
| End AA | | 661 | 661 | 200 | 200 | 200 | 162 | 163 | | | 160 | 166 | 163 | 171 | | | | 160 | | | | 160 |
| Start AA | | 53 | 30 | 59 | 29 | 53 | _ | - | | ļ | 7 | - | m | L | | | | 2 | | | | 2 |
| Chain ID | | ¥ | V | | | | | Ą | | | ∢ | | | 4 | | | | Ą | | | | ۷ |
| PDB CD | | Imf | lmfr | 2fha | 2fha | 2fha | 1858 | lawq | | | Iawq | Joh | Ich | Icyn | | | | lcyn | | | | ų y |
| S B S | | 541 | 541 | 541 | 541 | 2 | 246 | 546 | | 1 | 246 — | 546 | 546 | 246 | | | | 246 | | | | 546 |

| | | | | | | | | • | | | |
|-----------------|---|--|--|---|--|--|--|---|---|---|--|
| PDB annotation | TRANS ISOMERASE 3, ISOMERASE, ROTAMASE | COMPLEX (ISOMERASE/PEPTIDE) ISOMERASE, ROTAMASE, COMPLEX (ISOMERASE/PEPTIDE) | COMPLEX (ISOMERASE/PEPTIDE) ISOMERASE, ROTAMASE, COMPLEX (ISOMERASE/PEPTIDE) | PEPTIDYLPROLYL CIS-TRANS ISOMERASE, CYCLOPHILIN A, CYCLOSPORIN A, PEPTIDYL CIS- TRANS ISOMERASE | ISOMERASE USA-CYP, SNUCYP-20, CYCLOPHILIN, SNRNP, SPLICEOSOMAL | ISOMERASE USA-CYP, SNUCYP-20, CYCLOPHILIN, SNRNP, SPLICEOSOMAL | | | | TRANSCRIPTION REGULATION SIGMA70, RNA POLYMERASE SIGMA FACTOR, TRANSCRIPTION REGULATION | TRANSCRIPTION REGULATION PROTO-ONCOGENE, NUCLEAR |
| Coumpound | | CYCLOPHILIN A; CHAIN: A; SUCCINYL-ALA-PRO-ALA-P- NITROANILIDE; CHAIN: B; | CYCLOPHILIN A; CHAIN: A; SUCCINYL-ALA-PRO-ALA-P- NITROANILIDE; CHAIN: B; | CYCLOPHILIN; CHAIN: A; CYCLOSPORIN A; CHAIN: D; | SNUCYP-20; CHAIN: A; | SNUCYP-20; CHAIN: A; | COMPLEX (ISOMERASE/IMMUNOSUPP RESSANT) CYCLOPHILIN C COMPLEXED WITH CYCLOSPORIN A 2RMC 3 | COMPLEX (ISOMERASEIMMUNOSUPP RESSANT) CYCLOPHILIN C COMPLEXED WITH CYCLOSPORIN A 2RMC 3 | COMPLEX (ISOMERASEIMMUNOSUPP RESSANT) CYCLOPHILIN C COMPLEXED WITH CYCLOSPORIN A 2RMC 3 | RNA POLYMERASE PRIMARY SIGMA FACTOR; CHAIN: NULL; | TRANSCRIPTION FACTOR PML; CHAIN: NULL; |
| SeqFold | | 69.67 | | | | | | 94.18 | | | |
| PMF | | | 86.0 | _ | _ | 86.0 | _ | | - | 0:01 | 0.03 |
| Verify score | | | 0.47 | 0.56 | 0.57 | 0.31 | 9.0 | | 0.39 | 0.33 | -0.43 |
| PSI- BLAST | | 7.00E-41 | 7.00E-41 | 6.80E-33 | 1.70E-31 | 2.80E-36 | 3.40E-31 | 8.40E-41 | 8.40E-41 | 0.0028 | 3.40E-06 |
| End AA | | 163 | 162 | 160 | 160 | 951 | 091 | 172 | 171 | 335 | 363 |
| Start | | 2 | 3 | 2 | 2 | | 2 | 2 | 9 | 219 | 319 |
| Chain | | A | ¥ | ¥ | ٧ | ¥ | ₹ . | ٧ | ٧ | | |
| 10 B | | llop | Ilop | lqng | Iqoi | Iqoi | 2ттс | 2ттс | 2гтс | 1sig | 1bor |
| SEQ NO DE | | 546 | 546 | 546 | 546 | 546 | 546 | 546 | 546 | 548 | 549 |

| PDB annotation | BODIES (PODS), LEUKEMIA, 2 TRANSCRIPTION REGULATION | TRANSCRIPTION REGULATION PROTO-ONCOGENE, NUCLEAR BODIES (PODS), LEUKEMIA, 2 TRANSCRIPTION REGULATION | | IMMUNE SYSTEM KH DOMAIN, ALPHA-BETA FOLD, RNA-BINDING MOTIF | IMMUNE SYSTEM KH DOMAIN, ALPHA-BETA FOLD RNA-BINDING MOTIF | IMMUNE SYSTEM KH DOMAIN, ALPHA-BETA FOLD RNA-BINDING MOTIP | IMMUNE SYSTEM KH DOMAIN, ALPHA-BETA FOLD RNA-BINDING MOTIF | IMMUNE SYSTEM KH DOMAIN, ALPHA-BETA FOLD RNA-BINDING MOTIF | RNA BINDING PROTEIN/RNA ASTROCYTIC NOVA-LIKE RNA- BINDING PROTEIN; KIA DOMAIN, ALPHA-BETA FOLD, RNA-BINDING MOTIE, PROTEIN/RNA, 2 STRUCTIRE | LIGASE CBL, UBCH?, ZAP-70, E2, UBIQUITINE, B.; PROSPHORYLATION, 2 TYROSINE KINASE, UBIQUITINATION, PROTEIN DEGRADATION, | METAL BINDING PROTEIN RING |
|------------------|--|--|---|---|--|--|--|--|---|---|----------------------------|
| Coumpound | | TRANSCRIPTION FACTOR PML; CHAIN: NULL; | VIRUS EQUINE HERPES VIRUS-1 (C3HC4, OR RING DOMAIN) ICHC 3 (NMR, 1 STRUCTURE) ICHC 4 | NEURO-ONCOLOGICAL VENTRAL ANTIGEN I; CHAIN: A; | RNA-BINDING NEUROONCOLOGICAL VENTRAL ANTIGEN 2; CHAIN: A, B, C, D; | RNA-BINDING NEUROONCOLOGICAL VENTRAL ANTIGEN 2; CHAIN: A. B. C. D: | RNA-BINDING NEUROONCOLOGICAL VENTRAL ANTIGEN 2; CHAIN: A, B, C, D; | RNA-BINDING NEUROONCOLOGICAL VENTRAL ANTIGEN 2; CHAIN: A, B, C, D; | RNA-BINDING PROTEIN NOVA-2; CHAIN: A, B; 20- MER RNA HAIRPIN; CHAIN: C, D; | SIGNAL TRANSDUCTION PROTEIN CBL; CHAIN: A; ZAP-70 PEPTIDE; CHAIN: B; UBIQUITIN-CONJUGATING ENZYME E12-18 KDA | CDK-ACTIVATING KINASE |
| SeqFold score | | | | | | | | | | | |
| PMF score | | 0.16 | 8.0 | 86:0 | 0.95 | 0.88 | 66.0 | 66.0 | _ | 0.71 | 0.27 |
| Verify score | | -0.5 | -0.21 | 0.49 | 0.42 | 0.44 | 0.3 | 0.51 | 99.0 | 0.28 | -0.37 |
| PSI- BLAST | | 9.80E-09 | 3.40E-12 | 2.80E-14 | 2.80E-14 | 2.80E-05 | 4.20E-16 | 2.80E-15 | 8.40E-15 | 3.40E-13 | 0.00068 |
| End AA | | 366 | 370 | 104 | 104 | 901 | 104 | 104 | 601 | 370 | 363 |
| Start AA | | 321 | 321 | 39 | 39 | 39 | . 68 | 39 | 39 | 320 | 317 |
| Chain ID | | | | ¥ | V | В | ပ | Q | ∢ | ∢ | V |
| D G | | lbor | 1chc | 1dt4 | 1dtj | 1dtj | Idtj | 1dtj | lec6 | Ifbv | 1g25 |
| SEQ BO: | | 549 | 549 | 549 | 549 | 549 | 549 | 549 | 549 | 549 | 549 |

| | | _ | | -, | | | | | | _ | | _ | | | | | | | | | | | | | | | | | | | | | | | | |
|------------------|---------------------------|----------------|---|---------------------|--------------------------|------------------------|-------------------------------|-------------------------------|----------------------------|--------------------------------|-----------------|----------|-------------|--------------------|--------------------|---------------------|-----------------------|---------------------------|-------------------------|----------------------------|------------------------------|-----------------------|---------------------------|-------------------|---------------------|-------------|-----------------------------|------------------------|-----------------------------|---|---------------------------|--------------------------------|-----------------------------|----------|---|--------------------------------|
| PDB annotation | FINGER PROTEIN MATI: RING | FINGER (C3HC4) | METAL BINDING PROTEIN RING FINGER PROTEIN MATI; RING | PINGER (C3HC4) | RECOMBINATION ACTIVATING | PROTEIN 1; RAG1, V(D)J | RECOMBINATION, ANTIBODY, MAD. | RING FINGER, 2 ZINC BINUCLEAR | CLUSTER, ZINC FINGER, DNA- | RIBONUCLEOPROTEIN RNA-BINITRIC | PROTEIN IVIG 19 | | TRANCEEDASE | METHYLTRANSFERASE | | STRUCTURAL GENOMICS | HYPOTHETICAL PROTEIN, | METHANOCOCCUS JANNASCHII | TRANSFERASE SAM-BINDING | DOMAIN, BETA-BARREL, MIXED | ALPHA-BETA, HEXAMER, 2 DIMER | TRANSFERASE | (METHYLTRANSFERASE) COMT; | METHING THE ASSE, | MEINTELIKANSFEKASE, | DEGRADATION | METHYL TE ANGERT AGE CON TO | ADENOSYL-L-METHIONINE: | GLYCINE METHY! TRANSEED ASE | TOWN TOWN TOWN TOWN TOWN TOWN TOWN TOWN | COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) 21NC | FINGER, DNA-BINDING PROTEIN | | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC | INCER DIVIA DIVIDIATO DO COMO. |
| Coumpound | ASSEMBLY FACTOR MATI; | CHAIN: A; | ASSEMBLY FACTOR MATI; CHAIN: A: | RAGI: CHAIN: NIII.1 | í. | | | | | VIGILIN; IVIG 5 CHAIN: | NULL; IVIG 6 | | GLYCINE N- | METHYLTRANSFERASE; | CHAIN: A, B, C, D; | MJ0882; CHAIN: A; | | In many in the control of | HINKING ARGININE N. | CHAIN 1 2 4 4 CHAIN | CATECITO! 0, 4, 3, 6; | METING TO DESCRIPTION | CHAIN: NIII 1 . | 1000 | | | GLYCINE N- | METHYLTRANSFERASE; | CHAIN: A, B; | | ╌ | DUPLEX | OLIGONUCLEOTIDE | + | DUPLEX | _ |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | | | | _ | | | 1 | | | | | , a. C | 7 |
| PMF score | | 0.25 | | 61.0 | | | | | | | 1 | 1 | 0.29 | | 1 | _ | | 530 | 3 | _ | 170 | - | | | _ | 1 | 0.06 | _ | 1 | 1 | 10.01 | _ | | 0.01 | | |
| Verify score | | -0.18 | | 91.0 | | | | | | 69.0 | T | 7 | 5 5 | | 02.0 | 95.0 | | 0.12 | | | -0.07 | | | | | 100 | _ | | \dagger | 000 | _ | | | -0.43 0 | | |
| PSI- BLAST | | 1.40E-09 | | 5.10E-12 | | | | | 7. 0007 | 4.20E-10 | | 3 AND 16 | 3.40E-13 | | 8 500 00 | 60-2000 | | 5.60E-07 | | | 4.20E-09 | | | | | \$ 108-16 | _ | | | 1 70F-23 | _ | _ | | 8.50E-25 | | |
| End | | 365 | \$ | 262 | | | | | 2 | 5 | | 165 | 3 | | 991 | | 7 | 164 | | 7 | 82 | | _ | | | 165 | | | r | 490 | | _ | + | 247 | \dashv | |
| Start AA | | 321 | 512 | 216 | | _ | | | 36 | | | 20 | : | | 51 | | 1 | 34 | | 1 | 48 | | | | | 28 | _ | | | 410 | - | | 7 | 0 440 | \neg | |
| Chain ID | | V | | | | _ | | | | | | A | _ | | | | | _ | | 1 | | | | _ | | Ī | _ | | | | | | Ť | _ | \exists | |
| EQ G | | 1825 | Ē | | | _ | | _ | lvig | , | 1 | 1d2h | | 1 | Idus A | | 1 | l bogr | _ | | | | | | _ | Ixva A | | 1 | 1 | laih A | _ | | Jolh A | | \dashv | |
| SEQ B B SEQ | | 249 | 249 | : | | _ | | | 849 | | + | 223 | _ | - | 233 | | 553 | _ | | 563 | _ | _ | _ | | | 553 | - | 1 | 1 | 554 | _ | | 554 10 | _ | 1 | |

| PDB annotation | | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA | CRYSTAL STRUCTURE, COMPLEX | COMPLEY (ZINC ENICED DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | COVETAL STRICTLING COMPLEY | (ZINC FINGER/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) TFIIIA; 5S GENE; | NMR, TFIIIA, PROTEIN, DNA, | TRANSCRIPTION FACTOR, 5S RNA 2 | GENE, DINA BINDING PROTEIN, ZINC | (TRANSCRIPTION REGIL ATIONONA) | TRANSCRIPTION REGULATION | TRANSCRIPTION REGULATION, ADRI, ZINC FINGER, NMR | TRANSCRIPTION REGULATION | TRANSCRIPTION REGULATION, ADRI, ZINC FINGER, NMR | | | | | | TRANSCRIPTION INHIBITOR BETA- | PROPELLER | COMPLEX (GTP- BINDING/TRANSDUCER) BETA1, |
|-----------------|----------------------------|---|----------------------------|--------------------------------|-----------------------|--------------------------------|-------------------|--------------------------------|------------------------|----------------------------|-------------------|------------------------|----------------------------------|----------------------------|--------------------------------|----------------------------------|--------------------------------|--------------------------|---|--------------------------|---|-----------------------|-------------------|------------------|--------------------|------------------------|-------------------------------|------------------------------------|---|
| Coumpound | BINDING SITE; CHAIN: B, C; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | DNA: CHAIN: A B D E. | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | DNA; CHAIN: A, B, D, E; | PROTEIN: CHAIN: C E C: | INCIEM, CERMIN. C, F, G, | | TRANSCRIPTION FACTOR | IIIA; CHAIN: A; 5S RNA | GENE; CHAIN: E, F; | | | | ADRI; CHAIN: NULL; | | ADRI; CHAIN: NULL; | | COMPLEX(TRANSCRIPTION | TRAMTRACK PROTEIN | (TWO ZINC-FINGER | PEPTIDE) COMPLEXED | WITH ZDRP 3 DNA 2DRP 4 | TRANSCRIPTIONAL | REPRESSOR TUPI; CHAIN: A, B, C; | GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT- |
| SeqFold | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | -0.19 | | 0.50 | 0.32 | | | 0.04 | | | | 0.04 | | | | | | 0.24 | | 0 | | 0.89 | | | | | 0 | | -0.13 |
| Verify score | | 0.14 | | 0.27 | 77.0 | | | -0.21 | | | | -0.03 | | | _ | | | 0.04 | | -0.35 | | 0.01 | | • | | | -0.15 | | 0.11 |
| PSI- BLAST | | 1.00E-10 | | 1 705 12 | 1.705-12 | | | 5.10E-09 | | | | 3.40E-13 | | | | | | 5.10E-13 | | 1.70E-15 | | 2.80E-11 | | | | | 3.40E-15 | | 1.70E-11 |
| End | | 1032 | | 470 | } | | | 586 | | | | 470 | | | | | | 472 | | 553 | | 472 | | | | | 295 | | 352 |
| Start | | 9001 | | 443 | } | | | 096 | | | | 366 | | | _ | | | 409 | | 464 | | 401 | | | | | 30 | | 136 |
| Chain ID | | Ð | | e | | | | 9 | | | | Ą | | | | | | | | | | V | | | | | ٧ | | д |
| PDB ID | | lme y | | and | , × | | | Ime | <u>~</u> | | | 143 | | | | | | 2adr | | 2adr | | 2drp | | | | | lej. | | lgot |
| SEQ No. u | | 554 | | 25.4 | 5 | | | 554 | | | | 554 | | | | | | 554 | | 554 | | 554 | | _ | | floor | 555 | | 355 |

| | | | | | , | , | | | | | | | - |
|-----------------|---|--|--|---|---|---|---|---|---|---|---|---|-------------|
| PDB annotation | TRANSDUCIN BETA SUBUNTT. GAAMAAI, TRANSDUCIN GAMMA SUBUNTI: COMPLEX (GTP- BINDINCTRANSDUCER), O PROTEIN, HETEROTRIMER 2 SIGNAL TRANSDUCTION | REPLICATION DNA NUCLEOTIDE EXCISION REPAIR, UVRABC, HELICASE, 2 HYPERTHERMOSTABLE PROTEIN | HYDROLASE UVRB; MULTIDOMAIN PROTEIN | GENE REGULATION APO PROTEIN | GENE REGULATION APO PROTEIN | TRANSLATION YEAST INITIATION FACTOR 44, EIF4A; HELICASE, INITIATION FACTOR 44, DEAD-BOX PROTEIN | TRANSLATION EUKARYOTIC INITIATION FACTOR 4A; IF4A, HELICASE, DEAD-BOX PROTEIN | TRANSLATION EUKARYOTIC INITIATION FACTOR 4A; IF4A, HELICASE, DEAD-BOX PROTEIN | HELICASE HELICASE, RNA, HEPATITIS, HCV, ATPASE, NTPASE | HELICASE HELICASE, RNA, HEPATITIS, HCV, ATPASE, NTPASE | HELICASE HELICASE, RNA, HEPATITIS, HCV, ATPASE, NTPASE | GENE REGULATION EIF4A; TRANSLATION INITIATION, SACCHAROMYCES CEREVISIAE, DEAD BOX 2 PROTEIN FAMILY | TRANSFERASE |
| Coumpound | BETA, CHAIN: B, GT- GAMMA; CHAIN: G; | DNA NUCLEOTIDE EXCISION REPAIR ENZYME UVRB; CHAIN: A; | EXCINUCLEASE ABC SUBUNIT B; CHAIN: A; | EXCINUCLEASE UVRABC COMPONENT UVRB; CHAIN: A; | EXCINUCLEASE UVRABC COMPONENT UVRB; CHAIN: A: | EUKARYOTIC INITIATION FACTOR 4A; CHAIN: A; | YEAST INITIATION FACTOR 4A; CHAIN: A, B; | YEAST INITIATION FACTOR 4A; CHAIN: A, B; | HCV HELICASE; CHAIN: A, B; | HCV HELICASE; CHAIN: A, B; | HCV HELICASE; CHAIN: A, B; | TRANSLATION INITIATION FACTOR 4A; CHAIN: A; | GLYCINE N- |
| SeqFold | | | | | | | | | | | | | |
| PMF | | 0.59 | 0.95 | 0.64 | 0.87 | - | _ | | 0.19 | 0 | 0.05 | | 0.95 |
| Verify score | | 0.1 | 0.01 | 90.0 | -0.03 | 0.8 | 0.74 | 0.64 | 0.39 | -0.35 | -0.11 | 0.84 | 0.27 |
| PSI- BLAST | | 3.40E-14 | 3.40E-14 | 8.40E-47 | 1.50E-16 | 8.50E-45 | 1.70E-55 | 0 | 1.70E-06 | 5.60E-09 | 1.70E-06 | 1.70E-52 | 1.40E-18 |
| End | | 317 | 317 | 379 | 317 | 374 | 204 | 374 | 310 | 316 | 310 | 203 | 195 |
| Start | | 175 | 175 | 123 | 175 | 213 | I | - | 236 | 40 | 236 | | 65 |
| Chain | | 4 | V | A | V | V | ¥ | В | ٧ | Ą | æ | ¥ | A |
| PDB ED | | Ic4o | 142 E | X6PI | 1d9x | 1fuk | Ifm | 1fuu | 1hei | Ihei | 1hei | 1qde | 1d2h |
| SEQ No: D | | 557 | 557 | 257 | 257 | 557 | 257 | 557 | 557 | 257 | 557 | 557 | 558 |

| PDB annotation | METHYLTRANSFERASE | TRANSFERASE METHYLTRANSFERASE | STRUCTURAL GENOMICS HYPOTHETICAL PROTEIN, METHANOCOCCUS JANNASCHII | STRUCTURAL GENOMICS HYPOTHETICAL PROTEIN, METHANOCOCCUS JANNASCHII | TRANSFERASE SAM-BINDING DOMAIN, BETA-BARREL, MIXED ALPHA-BETA, HEXAMER, 2 DIMER | METHYLTRANSFERASE GNMT, S- ADENOSYL-L-METHIONINE: GLYCINE METHYLTRANSFERASE | METHYLTRANSFERASE ERMAM; METHYLTRANSFERASE, ERM, ERMAM, MLS ANTIBIOTICS, NMR, 2 RRNA | METHYLTRANSFERASE TRANSFERASE, METHYLTRANSFERASE, RESTRICTION SYSTEM | HYDROLASE PROTEIN-TYROSINE PHOSPHATASE, HYDROLASE, PROTEIN TYROSINE PHOSPHATASE, CATALYTIC DOMAIN, 2 WPD LOOP, SH2 DOMAIN | HYDROLASE DUAL SPECIFICITY PHOSPHATASE, MAP KINASE HYDROLASE | HYDROLASE DUAL SPECIFICITY PHOSPHATASE, MAP KINASE HYDROLASE | HYDROLASE VHR; HYDROLASE, PROTEIN DUAL-SPECIFICITY PHOSPHATASP | HYDROLASE VHR; HYDROLASE, |
|------------------|--|--|--|--|---|---|---|---|---|--|--|--|---------------------------|
| Coumpound | METHYLTRANSFERASE; CHAIN: A, B, C, D; | GLYCINE N- METHYLTRANSFERASE; CHAIN: A. B. C. D; | MJ0882; CHAIN: A; | MJ0882; CHAIN: A; | HNRNP ARGININE N. METHYLTRANSFERASE; CHAIN: 1, 2, 3, 4, 5, 6; | GLYCINE N- METHYLTRANSFERASE; CHAIN: A, B; | RRNA METHYLTRANSFERASE; CHAIN: NULL; | ADENINE-N6-DNA- METHYLTRANSFERASE TAQI; CHAIN: A, B; | SHP-1; CHAIN: NULL; | PYST1; CHAIN: NULL; | PYSTI; CHAIN: NULL; | HUMAN VHI-RELATED DUAL-SPECIFICITY PHOSPHATASE CHAIN: A B: | HUMAN VHI-RELATED |
| ScqFold score | | | | | | | | | | 137.8 | | 96.19 | |
| PMF | | 0.19 | 0.89 | 0.93 | 0.31 | 0.72 | 0.06 | 0.48 | 0.25 | | | | _ |
| Verify | | -0.17 | 0.35 | 0.25 | 0.11 | -0.08 | 0.44 | 0.09 | -0.17 | | 0.88 | | 0.78 |
| PSI- BLAST | | 2.80E-13 | 1.40E-12 | 2.80E-14 | 1.70E-26 | 5.10E-21 | 1.20E-06 | 1.20E-08 | 4.20E-05 | 3.40E-39 | 3.40E-39 | 1.10E-34 | 1.10E-34 |
| End | | 223 | 187 | 213 | | 195 | 157 | 681 | 301 | 298 | 287 | 307 | 298 |
| Start AA | | 19 | 89 | 83 | 43 | 43 | 71 | 79 | 225 | 158 | 129 | 135 | 142 |
| Chain ID | | ٧ | 4 | 4 | _ | ٧ | , | Ą | | | | ¥ | V |
| PDB UD | | 142h | Idus | Idus | 1g6q | Ixva | lyub | 2ad m | lgwz | Ĭ d | 単 d | lvhr | Jvþr |
| SEQ ID NO: | | 558 | 558 | 558 | 558 | 558 | 258 | 558 | 529 | 529 | 559. | 529 | 529 |

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|------------------|---|--|---|---|---|---|---|--|--|--|---|
| PDB annotation | PROTEIN DUAL-SPECIFICITY PHOSPHATASE | HYDROLASE VHR, HYDROLASE, PROTEIN DUAL-SPECIFICITY PHOSPHATASE | | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX |
| Coumpound | DUAL-SPECIFICITY PHOSPHATASE CHAIN: A, B; | HUMAN VHI-RELATED DUAL-SPECIFICITY PHOSPHATASE CHAIN: A, B; | | QGSK ZINC FINGER PEPTIDE, CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B, C: | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | QGSR ZINC FINGER PEPTIDE, CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B. C. | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A. B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; |
| SeqFold score | | | | | | 56.74 | | | | 69.14 | |
| PMF | | _ | | 0.77 | 0.83 | | 0.86 | 69:0 | | | 0.46 |
| Verify | | 0.29 | | 0.4 | 0.03 | | -0.45 | 0.07 | 0.08 | | -0.37 |
| PSI- BLAST | | 1.00E-32 | | 6.80E-22 | 1.50E-28 | 1.50E-28 | 1.20E-24 | 6.80E-36 | 5.10E-49 | 5.10E-49 | 3.40E-40 |
| End | | 282 | | 248 | 276 | 278 | 288 | 246 | 276 | 277 | 288 |
| Start AA | | 146 | | 188 | 194 | 194 | 222 | 187 | 193 | 193 | 221 |
| Chain | | Ą | | ¥ | ¥ | ¥ | ∢ | ပ | ပ | O | ပ |
| PDB U | | lvhr | | lalh | lalh | lalh | lalh | J me | Jme y | y Jmc | J me |
| SEQ B B SE | | | | 999 | 999 | 999 | 999 | 996 | 366 | 999 | 999 |

| | _ | | | | | _ | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----------------|-------------------|---|--|--|--|--------------------------------|---|--------------------------------|------------------------|----------------------------------|---------------------------------|-------------------------------|------------------|--------------------------------|-------------------------|-------------------------|--------------------|----------------------|------------------------------|------------------------|------------------------------|---------------------------|--------------------------------|-----------------------------|------------------------|------------------------|-------------------------------|---------------------------|--------------------------------|-----------------------------|---|------------------------|
| PDB annotation | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (TRANSCRIPTION BEGYLL A FLOMENA) TEHLA SE CENE | NECOCALIONDINA) ITHIR, 35 CENE, NMR, TFIIIA, PROTEIN, DNA, | TRANSCRIPTION FACTOR, 5S RNA 2 | GENE, DINA BINDING PROTEIN, ZINC FINGER, COMPLEX 3 | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) IFIIIA; 35 GENE; | THE ANICODITION EACTOR SCIDIA 2 | GENE DNA BINDING PROTEIN ZING | FINGER COMPLEX 3 | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX | (TRANSCRIPTION | REGULATION/DNA), RNA | NUTATION 2INC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | COMPLEY OF ANSCRIPTION | REGILLATION/DNA) YING-YANG 1: | TRANSCRIPTION INITIATION. | INITIATOR ELEMENT, YYI, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX TREADS BETTON BEGIN ATTONIONAL TO A SHIP AND A STONIONAL TO A SHIP A SHIP TO A SHIP | COMPLEX (TRANSCRIPTION |
| Coumpound | | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | , | TRANSCRIPTION FACTOR | GENE; CHAIN: E, F; | | | | TRANSCRIPTION FACTOR | IIIA; CHAIN: A; SS KNA | GENE, CHAIN: E, F; | | | | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | | | YYI: CHAIN: C: ADENO- | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | VVI. CHANI. C. ADENO | ASSOCIATED VIRIS P5 | INITIATOR ELEMENT DNA: | CHAIN: A, B; | | | YY1: CHAIN: C; ADENO- |
| SeqFold | | | | 50.62 | | | | | | | | | | | | | | | | 56.56 | | | | | | | | | | | | |
| PMF | | 0.92 | | | | | | | 10:0 | | | | | | 0.16 | | | | | | | | | | | 08.0 | 6.9 | | | | | 0.88 |
| Verify score | | -0.03 | | | | | | | -0.15 | | | | | | -0.28 | | | | | | | | | | | -0.33 | 20.32 | | | | | -0.02 |
| PSI- BLAST | | 1.70E-13 | | 6.80E-18 | | | | | 6.80E-18 | | | | | | 1.40E-20 | | | | | 6.80E-29 | | | | | | 6 905 30 | 0.005-27 | | | | | 5.10E-27 |
| End | | 246 | | 280 | | | | | 276 | | | | | | 277 | | | | | 277 | | | | | | 276 | 0/7 | | | | | 284 |
| Start | | 219 | | 193 | | | | | 194 | | | | | | 861 | | | | | 167 | | | | | | 186 | 201 | | | | | 201 |
| Chain | | 9 | | ¥ | | | | | ٧ | | | | | | γ | | | | | O | | | | | | L | | | | | | O |
| PDB | | y Ime | | <u> </u> | | | | | 9 | | | | | | 1466 | | | | | Pgal | | | | | | Mil | 3 | | | | | 566 1ubd |
| SEQ B B SS | | 999 | | 999 | | | | | 999 | | | | | | 995 | | | | | 266 | | | | | | 3,75 | 3 | | | | | 999 |

| PDB annotation | REGULATIONDNA) YING-YANG 1: TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINIDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | SCAFFOLD PROTEIN SCAFFOLD PROTEIN, PPZA, PHOSPHORYLATION, HEAT REPEAT | SCAFFOLD PROTEIN SCAFFOLD PROTEIN, PP2A, PHOSPHORYLATION, HEAT REPEAT | TRANSPORT PROTEIN SERINE-RICH RNA POLYMERASE I SUPPRESSOR PROTEIN; ARM REPEAT | TRANSPORT PROTEIN SERINE-RICH RNA POLYMERASE I SUPPRESSOR PROTEIN; ARM REPEAT | TRANSPORT PROTEIN SERINE-RICH RNA POLYMERASE I SUPPRESSOR PROTEIN; ARM REPEAT | TRANSPORT PROTEIN SERINE-RICH RNA POLYMERASE I SUPPRESSOR PROTEIN; ARM REPEAT | NUCLEAR IMPORT RECEPTOR KARYOPHERIN ALPHA; NUCLEAR IMPORT RECEPTOR, NUCLEAR LOCALIZATION SIGNAL, 2 |
|-----------------|--|---|---|---|---|--|--|--|--|--|
| Соитроинд | ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | PROTEIN PHOSPHATASE PP2A; CHAIN: A, B; | PROTEIN PHOSPHATASE PP2A; CHAIN: A, B; | KARYOPHERIN ALPHA; CHAIN: A, B; MYC PROTO- ONCOGENE PROTEIN; CHAIN: C, D, E, F; | KARYOPHERIN ALPHA; CHAIN: A. B; MYC PROTO- ONCOGENE PROTEIN; CHAIN: C, D, E, F; | KARYOPHERIN ALPHA; CHAIN: A, B; MYC PROTO- ONCOGENE PROTEIN; CHAIN: C, D. E. F. | KARYOPHERIN ALPHA; CHAIN: A, B, MYC PROTO- ONCOGENE PROTEIN; CHAIN: C, D, E, F: | IMPORTIN ALPHA; CHAIN: A; |
| SeqFold | | 57.42 | | 161.25 | | | ٠ | | | |
| PMF | | | 0.72 | | 0.71 | - | 0.83 | _ | - | 96:0 |
| Verify score | | | 0.23 | | -0.03 | 0.42 | 90:0- | 0.44 | 0.34 | 0.38 |
| PSI- BLAST | | 1.50E-26 | 1.50E-26 | 1.70E-40 | 1.70E-40 | 1.30E-43 | 1.40E-31 | 1.70E-37 | 3,40E-28 | 5.10E-21 |
| End AA | | 278 | 278 | 509 | 509 | 905 | 459 | 109 | 390 | 603 |
| Start | | 133 | 188 | _ | 6 | 144 | 81 | 184 | 7 | 304 |
| Chain 10 | | < | ∢ | ¥ | Ą | 4 | ∢ | ∢ | ∢. | ¥ |
| 808 01 | | 2gli | 2gli | 1b3u | Ib3u | lee4 | lee4 | lee4 | lee4 | lial |
| S a S | | 999 | 995 | 571 | 125 | 172 | 172 | 571 | 172 | 571 |

| PDB annotation | ARMADILLO REPEATS, AUTOINHIBITION, INTRASTERIC REGULATION | NUCLEAR IMPORT RECEPTOR KARYOPHERN MALHA, NUCLEAR IMPORT RECEPTOR, NUCLEAR LOCALIZATION SIGNAL, 2 ARMADILLO REPEATS, AUTOINHISTION, INTRASTERIC | NUCLEAR IMPORT RECEPTOR KARYOPHERM NATHA, NUCLEAR LAFORT RECEPTOR, NUCLEAR LOCALIZATION SIGNAL, 2 ARMADILLO REPEATS, AUTOINHIBITION, INTRASTERIC | NUCLEAR IMPORT RECEPTOR KARYOPRERN MALEHA, NUCLEAR IMPORT RECEPTOR, NUCLEAR LOCALIZATION SIGNAL, 2 ARMADILLO REPEATS, AUTOINHIBITION, INTRASTERIC | SMALL GTPASE KARYOPHERIN BETA, P95 SMALL GTPASE, NUCLEAR TRANSPORT RECEPTOR | SMALL GTPASE KARYOPHERIN BETA, P95 SMALL GTPASE, NUCLEAR TRANSPORT RECEPTOR | NUCLEAR TRANSPORT PROTEIN COMPLEX HEAT REPEATS, NUCLEAR TRANSPORT PROTEIN COMPLEX | TRANSFORT RECEPTOR KARYOPHERN BETA-I, NUCLEAR FACTOR P97, IMPORTIN IMPORTIN ALPHA-2 SUBINIT, KARYOPHERIN ALPHA-2 SUBONIT, KARYOPHERIN ALPHA-2 TRANSFORT RECEPTOR, NUCLEAR IMPORT, HEAT MOTIF, NY SENDING | STRUCTURAL PROTEIN ARMADILLO |
|-----------------|---|---|--|---|---|---|---|--|------------------------------|
| Coumpound | | IMPORTIN ALPHA; CHAIN: A; | IMPORTIN ALPHA; CHAIN: A; | IMPORTIN ALPHA; CHAIN: A; | RAN; CHAIN: A, C; IMPORTIN BETA SUBUNIT; CHAIN: B, D; | RAN; CHAIN: A, C; IMPORTIN BETA SUBUNIT; CHAIN: B, D; | KARYOPHERIN BETA2; CHAIN: B; RAN; CHAIN: C; | IMPORTIN BETA SUBUNIT; CHAIN: A; IMPORTIN ALPHA-2 SUBUNIT; CHAIN: B; | BETA-CATENIN; CHAIN: |
| SeqFold | | 152.5 | | | | | | | |
| PMF | | | 0.19 | 0.88 | 0.4 | -0.09 | 0.74 | 0.16 | 0.64 |
| Verify score | | | 0.26 | 0.18 | -0.01 | 0.11 | 10.0 | -0.16 | 0.29 |
| PSI- BLAST | | 1.40E-32 | 1.70E-09 | 1.40E-32 | 6.80E-13 | 5.10E-12 | 3.40E-49 | 6.80E-23 | 1.40E-22 |
| End AA | | 475 | 607 | 390 | 909 | 26 | 909 | 474 | 200 |
| Start | | 33 | 530 | 7 | 225 | 3 | 9 | m | 80 |
| Chain | | ∢ | ⋖ | ∢ | _α | øq. | en en | ∢ | |
| 20.8 CD | | lial | lial | Lial | libr | libr | 1qbk | logr | 2bct |
| Se o Se | | 571 | 571 | 271 | 571 | 57.1 | 571 | 241 | 571 |

| | | | | | | | | | _ | | | | |
|------------------|---|---|---|---|---|---|---|---|---|--|--|--|---|
| PDB annotation | REPEAT, BETA-CATENIN, STRUCTURAL PROTEIN | STRUCTURAL PROTEIN ARMADILLO REPEAT, BETA-CATENIN, STRUCTURAL PROTEIN | STRUCTURAL PROTEIN ARMADILLO REPEAT, BETA-CATENIN, STRUCTURAL PROTEIN | STRUCTURAL PROTEIN ARMADILLO REPEAT, BETA-CATENIN, STRUCTURAL PROTEIN | ARMADILLO REPEAT ARMADILLO REPEAT, BETA-CATENIN, CYTOSKELETON | | LIPID TRANSPORT APO A-I; LIPOPROTEIN, LIPD TRANSPORT, CHOLESTEROL METABOLISM, 2 ATHENOSCLEROSIS, HDL, LCAT- ACITYATION | STRUCTURAL PROTEIN TWO REPEATS OF SPECTRIN, ALPHA HELICAL LINKER REGION, 22 TANDEM 3-HELIX COLED-COLLS, STRUCTURAL PROTEIN | CONTRACTILE PROTEIN TRIPLE. HELIX COILED COIL, CONTRACTILE PROTEIN | TRANSCRIPTION REGULATION SIGMA70; RNA POLYMERASE SIGMA FACTOR, TRANSCRIPTION REGULATION |
| Coumpound | NULL; | BETA-CATENIN; CHAIN: NULL; | BETA-CATENIN; CHAIN: . NULL; | BETA-CATENIN; CHAIN: NULL; | BETA-CATENIN; CHAIN: NULL; | BETA-CATENIN; CHAIN: NULL; | BETA-CATENIN; CHAIN: NULL; | BETA-CATENIN; CHAIN: NULL; | | APOLIPOPROTEIN A-1; CHAIN: A, B, C, D; | ALPHA SPECTRIN; CHAIN: A, B, C, | HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A; | RNA POLYMERASE PRIMARY SIGMA FACTOR; CHAIN: NULL; |
| SeqFold score | | 160.13 | | | | 141.33 | | | | 67.34 | 62.14 | 67.92 | |
| PMF | | | I | 0.94 | -1.41 | | 1202.08 | 1 | | | | | 0.07 |
| Verify score | | | 0.39 | 0.31 | 0.57 | | 0.45 | 0.35 | | | · | | -0.28 |
| PSI- BLAST | | 6.80E-44 | 8.40E-25 | 6.80E-44 | 6.80E-18 | 1.40E-31 | 5.10E-36 | 1.40E-31 | | 5.60E-11 | 2.80E-12 | 1.40E-13 | 2.80E-09 |
| End AA | | 607 | 431 | 607 | 386 | 476 | 604 | 430 | | 219 | 219 | 245 | 161 |
| Start | | 68 | 6 | 16 | - | | 138 | 21 | | EZ | 9 | e a | 31 |
| Chain 190 | | | | | | | | | | V | ⋖ | ∢ | |
| 803 ED | | 2pct | 2pct | 2bct | 3bct | 3bct | 3bct | 3bct | | lavi | lcun | Iqui | lsig |
| S e S | | 571 | 57.1 | 57.1 | 57.1 | 571 | 571 | 571 | | 572 | 572 | 272 | 572 |

| | | | | | • | | | | , |
|-----------------|--|--|---|---|--|--|--|---|---|
| PDB annotation | LIPID TRANSPORT APO A-1; LIPOPROTEIN, LIPID TRANSPORT, CHOLESTEROL, METABOLISM, 2 ATHEROSCLEROSIS, HDL, LCAT- ACTIVATION | TRANSMEMBRANE PROTEIN COLICIN, BACTERIOCIN, ION CHANNEL FORMATION, TRANSMEMBRANE 2 PROTEIN | STRUCTURAL PROTEIN TWO REPEATS OF SPECTRIN, ALPHA HELICAL LINKER REGION, 2.2 TANDEM 3-HELIX COLED-COILS, STRUCTURAL PROTEIN | STRUCTURAL PROTEIN TWO REPEATS OF SPECTRIN, ALPHA HELICAL LINKER REGION, 22 TANDEM 3-HELIX COLLED-COLLS, STRUCTURAL PROTEIN | SIGNALING PROTEIN GUANINE NUCLEOTINE, BINDING PROTEIN I; GBP, GTP HYDROLYSIS, GDP, GMP, INTERFERON INDUCED, DYNAMIN 2 RELATIED, LARGE GTPASE FAMILY, SIGNALING PROTEIN | ENDOCYTOSIS/EXOCYTOSIS NSECI; PROTEIN-PROTEIN COMPLEX, MULTI-SUBUNIT | ENDOCYTOSIS/EXOCYTOSIS NSECI; PROTEIN-PROTEIN COMPLEX, MULTI-SUBUNIT | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGMIN ASSOCIATED 35 KDA PROTEIN, P35A, THREE HELIX BUNDLE | SIGNALING PROTEIN GBP, GTP HYDROLYSIS, GDP, GMP, INTERFERON INDUCED, DYNAMIN 2 RELATED, LANGE GTPASE FAMILY. GMPNP, GPPNHP. |
| Coumpound | APOLIPOPROTEIN A-1; CHAIN: A, B, C, D; | COLICIN IA; CHAIN: NULL; | ALPHA SPECTRIN; CHAIN: A, B, C; | ALPHA SPECTRIN; CHAIN: A, B, C; | INTERFERON-INDUCED GUANYLATE-BINDING PROTEIN 1; CHAIN: A; | SYNTAXIN BINDING PROTEIN 1; CHAIN: A; SYNTAXIN 1A; CHAIN: B; | SYNTAXIN BINDING PROTEIN 1; CHAIN: A; SYNTAXIN 1A; CHAIN: B; | SYNTAXIN-1A; CHAIN: A, B, C; | INTERFERON-INDUCED GUANYLATE-BINDING PROTEIN I; CHAIN: A; |
| SeqFold | | | | | | | | | |
| PMF | -0.18 | -0.2 | -0.01 | -0.12 | -0.13 · | -0.17 | -0.19 | -0.18 | -0.19 |
| Verify score | 0.52 | 90:00 | 0.5 | 0.57 | 0.43 | 0.39 | 0.31 | 0.43 | 0.29 |
| PSI- BLAST | 7.00E-13 | 4.20E-16 | 5.60E-12 | 7.00E-15 | 1.40E-10 | 8.40E-14 | 1.40E-11 | 1.10E-16 | 4.20E-11 |
| End | 137 | 175 | 5/1 | 125 | 140 | 145 | 175 | 129 | 145 |
| Start AA | | 7 | - | 9 | 16 | 4 | ∞ | . 41 | = |
| Chain TD | 4 | | V | ¥ | ∢ | В | В | ٧ | ¥ |
| 808 00 | lavi | lcii | lcun | lcun | 1dg3 | 1dn1 | ldn1 | lez3 | IŚu |
| SEQ BO: | 573 | 573 | 573 | 573 | 573 | 573 | 573 | 573 | 573 |

| | | | | | | _ | | | | | | | |
|-------------------|--|--|--|--|--|---|---|---|--|---|---|---|-------------------------------|
| PDB annotation | PROTEIN TRANSPORT HELLX-TURN- HELLX TPR-LIKE REPEAT, PROTEIN TRANSPORT | CONTRACTILE PROTEIN TRIPLE- HELIX COILED COIL, CONTRACTILE PROTEIN | CONTRACTILE PROTEIN TRIPLE- HELIX COILED COIL, CONTRACTILE PROTEIN | CONTRACTILE PROTEIN TRIPLE- HELIX COILED COIL, CONTRACTILE PROTEIN | COMPLEASON CTRONS CTRON | | TOXIN BINDING PROTEIN TWO DOMAINS: BETA PROPELLER AND ALPHA/BETA FOLD | TOXIN BINDING PROTEIN TWO DOMAINS: BETA PROPELLER AND ALPHA/BETA FOLD | TOXIN BINDING PROTEIN TWO DOMAINS: BETA PROPELLER AND ALPHABETA FOLD | TOXIN BINDING PROTEIN TWO DOMAINS: BETA PROPELLER AND ALPHA/BETA FOLD | TOXIN BINDING PROTEIN TWO DOMAINS: BETA PROPELLER AND ALPHA/BETA FOLD | TRANSCRIPTION INHIBITOR BETA- PROPELLER | TRANSCRIPTION INHIBITOR BETA- |
| Coumpound | VESICULAR TRANSPORT PROTEIN SEC17; CHAIN: A; | HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A; | HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A; | HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A; | TRANSDICIN; CHAIN: B. G. PHOSDUCIN; CHAIN: P, | | TOLB PROTEIN; CHAIN: A; | TOLB PROTEIN; CHAIN: A; | TOLB PROTEIN; CHAIN: A; | TOLB PROTEIN; CHAIN: A; | TOLB PROTEIN; CHAIN: A; | TRANSCRIPTIONAL REPRESSOR TUP1; CHAIN: A, B, C; | TRANSCRIPTIONAL |
| SeqFold score | | | 53.17 | | | | | | | | | | |
| PMF | -0.2 | -0.2 | | -0.18 | -0.19 | | 0.22 | 0.1 | 0 | 0.22 | -0.12 | -0.14 | |
| Verify score | 0.2 | 0.4 | | 0.36 | 0.08 | | 0.47 | 0.37 | 0.41 | -0.14 | 0.22 | 9.14 | 8.0 |
| PSI- BLAST | 1.40E-12 | 5.60E-12 | 1.40E-19 | 1.40E-19 | 8.40E-11 | | 9.80E-18 | 5.60E-16 | 4.20E-15 | 5.10E-05 | 1.40E-09 | 5.60E-91 | 1.70E-76 |
| End | 146 | 101 | 250 | 174 | 144 | | 358 | 466 | 484 | 476 | 209 | 484 | 484 |
| Start AA | 9 | - | 9 . | 7 | 7 | | 110 | 172 | 262 | 353 | . 16 | 109 | 193 |
| Chain ID | ٧ | ¥ | ¥ | ¥ | Q. | | Ą | A | Ą | ¥ | V | ∢ | < |
| PDB CD | lqqe | Iquu | lquı | lquu | 2trc | | lcrz | lcrz | lcrz | lcrz | lorz | lerj | leri |
| SEQ No. to SEQ | 573 | 573 | 573 | 573 | 573 | | 574 | 574 | 574 | 574 | 574 | 574 | 574 |

| PDB annotation | PROPELLER | TRANSCRIPTION INHIBITOR BETA- PROPELLER | COMPLEX (GTP- BINDINGTRANSDUCER) BETA1, TRANSDUCTN BETA SUBUIT; GAMAA1, TRANSDUCTN GAMMA SUBUNIT; COMPLEX (GTP- BINDINGTRANSDUCER), GP HETEROTRINER 2 SIGNAL | COMPLEX (GTP. BINDINGTRANSDUCER) BETA1, TRANSDUCIN BETA SUBUNT; GAMAAI, TRANSDUCIN GAMAA SUBUNT; COMPLEX (GTP. BINDINGTRANSDUCER), G PROTEIN, HETEROTRANSDUCTION | COMPLEX (GTP- BINDING/TRANSDUCER, BETA1, TRANSDUCIN BETA SUBINIT; GAMMA, TRANSDUCIN GAMMA SUBJANT; COMPLEX (GTP- BINDING/TRANSDUCER), G PROTEIN, HETEROTRINER 2 SIGNAL | COMPLEX (GTP. BINDING/TRANSDUCER, BETAI, TRANSDUCIN BETA SUBUNIT; GAMAAI, TRANSDUCIN GAMMA SUBUNIT; COMPLEX (GTP. BINDING/TRANSDUCER), G PROTEIN, HETERORIAMER 2 SIGNAL | COMPLEX (GTP- BINDING/TRANSDUCER) BETA1, TRANSDUCIN BETA SUBUNIT; GAMMA1, TRANSDUCIN GAMMA |
|------------------|------------------------------------|---|--|--|--|---|---|
| Coumpound | REPRESSOR TUP1; CHAIN: A, B, C; | TRANSCRIPTIONAL REPRESSOR TUPI; CHAIN: A, B, C; | GT-ALPHA/GI-ALPHA CHMERA, CHANI: A; GT- BETA, CHANI: B; GT- GAMMA; CHANI: G; | GT-ALPHA/GI-ALPHA CHMERA, CHAN: A; GT- BETA; CHAN: B; GT- GAMMA; CHAN: G; | GT-ALPHA/GI-ALPHA CHINERA, CHARIN A; GT- BETA, CHAIN: B; GT- GAMMA; CHAIN: G; | GT-ALPHA/GI-ALPHA CHINERA, CHARIN: A; GT- BETA; CHARN: B; GT- GAMMA; CHAIN: G; | GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT- BETA; CHAIN: B; GT- GAMMA; CHAIN: G; |
| ScqFold score | | | | | | | 150.13 |
| PMF | | _ | - | - | _ | 66:0 | |
| Verify score | | 0.46 | 0.95 | 0.7 | 0.79 | 0.43 | |
| PSI- BLAST | | 1.70E-67 | 3.40E-71 | 1.00E-50 | 6.80E-79 | 3.40E-55 | 3.40E-71 |
| End | | 356 | 400 | 273 | 483 | 315 | 400 |
| Start | | 48 | 101 | 115 | 190 | 45 | 92 |
| Chain | | V | æ | Д | æ | æ | В |
| PDB DD | | jej. | lgot | Igot | lgot | lgot | Igot |
| SEQ NO: | | 574 | 574 | 574 | 574 | 574 | 574 |

| PDB annotation | SUBUNIT, COMPLEX (GTP- BINDING/TRANSDUCER), G PROTEIN, HETEROTRIMER 2 SIGNAL TRANSDUCTION | HYDROLLASE PROLYL ENDOPEPTIDASE, POST-PROLINE CLEAVING PROLYL OLIGOPEPTIDASE, AANESIA, ALPHAGETA-HYDROLASE, BETA-2 PROPELLER | OXIDOREDUCTASE ENZYME, NITRITE REDUCTASE, OXIDOREDUCTASE, DENITRIFICATION, 2 ELECTRON TRANSPORT, PERIPLASMIC | TRANSMEMBRANE PROTEIN COLICIN, BACTERIOCIN, ION CHANNEL FORMATION, TRANSMEMBRANE 2 PROTEIN | | | | ٠ | INSECT IMMUNITY INSECT IMMUNITY, LPS-BINDING, HOMOPHIJC ADHESION | INSECT IMMUNITY INSECT IMMUNITY, LPS-BINDING, HOMOPHILIC ADHESION | RECEPTOR RECEPTOR, SIGNAL TRANSDUCER OF IL-6 TYPE CYTOKINES, THIRD 2 N-TERMINAL DOMAIN, TRANSMEMBRANE, GLYCOPROTEIN | T-CELL SURFACE GLYCOPROTEIN IMMUNOGLOBULIN FOLD, |
|----------------|--|--|--|---|----------------------|---------------------------------|--------------------------------------|---------------------------------------|--|---|---|--|
| Coumpound | | PROLYL OLIGOPEPTIDASE; CHAIN: A; | CYTOCHROME CDI NITRITE REDUCTASE, CHAIN: A, B; | COLICIN IA; CHAIN: NULL; | 411 124 1 1101 11101 | DEFENSIN DEFENSIN/HNP3-3 IDFN 3 | DEFENSIN DEFENSIN /HNPS- 3 IDFN 3 | DEFENSIN DEFENSIN /HNP\$- 3 IDFN 3 | HEMOLIN; CHAIN: A, B; | HEMOLIN; CHAIN: A, B; | GP130; CHAIN: NULL; | T-CELL SURFACE GLYCOPROTEIN CD4; |
| SeqFold | | | | 98.21 | 200 | 26:60 | | | 111.17 | | | |
| PMF | | 0.05 | -0.19 | | | | _ | _ | | 0.05 | 90.0- | -0.01 |
| Verify | | -0.33 | 0.43 | | | | -0.35 | -0.35 | | 0 | 0.22 | 0.43 |
| PSI- BLAST | | 0.00056 | 5.60E-79 | 1.70E-10 | 0.00 | 1.105-12 | 1.10E-12 | 5.10E-11 | 1.70E-47 | 1.70E-47 | 5.60E-11 | 1.40E-19 |
| End | | 172 | 478 | 648 | 3 | 101 | 101 | 101 | 435 | 416 | 434 | 220 |
| Start AA | | Ξ | 104 | 49 | | 7/ | 73 | 73 | 30 | 32 | 344 | 49 |
| Chain | | ∢ | < | | | A | ٧ | Ą | Α | 4 | | |
| EDB DD | | 1qfm | 1 _p l | lcii | ٤ | He He | 1dfn | 1dfn | 1bih | lbih | lbj8 | lcdy |
| SEQ NO. | | 574 | 574 | 575 | 100 | 3// | 577 | 577 | 578 | 878 | 578 | 578 |

| . PDB annotation | TRANSMEMBRANE, GLYCOPROTEIN, T-CELL, 2 MHC, LIPOPROTEIN, T- CELL SURFACE GLYCOPROTEIN | | CELL ADHESION NEURAL CELL ADHESION | CELL ADHESION NEURAL CELL ADHESION | IMMUNE SYSTEM ABZYME TRANSITION STATE ANALOG, IMMUNE SYSTEM | GROWTH FACTOR/GROWTH FACTOR RECEPTOR FGE, FGFR IMMUNOGLOBULIN-LIKE, SIGNAL TRANSDUCTION, 2 DIMERIZATION GROWTH FACTOR/GROWTH FACTOR RECEPTOR | GROWH FACTORORDY FACTOR RECEPTOR FGF, FGFR FROM INMUNOCIOBULIN-LIKE, SIGNAL TRANSDUCTION, 2 DIMERIZATION GROWTH FACTOR GROWTH FACTOR GROWTH FACTOR FA | GROWTH FACTOR/GROWTH FACTOR REGEPTOR FGF, FGFR, IMMUNGGLOBULIN-LIKE, SIGNAL TRANSDUCTION, 2 DIMERIZATION GROWTH FACTOR/GROWTH FACTOR RECEPTOR | CELL ADHESION NCAM; IMMUNOGLOBULIN FOLD, GLYCOPROTEIN |
|------------------|---|--|------------------------------------|------------------------------------|--|--|--|--|---|
| Соитроинд | CHAIN: NULL; | NEURAL ADHESION MOLECULE BROSOPHILA MOLECULE BROSOPHILA (CHYMOTRYPTIC FRAGMENT CONTAINNG THE ICEB 3 TWO AMINO PROXIMAL FIBRONECTIN TYPE III REPEATS I CFB 5 (RESIDUES 610 - 814) I CFB 5 | AXONIN-1; CHAIN: A; | AXONIN-1; CHAIN: A; | 7C8 FAB FRAGMENT; SHORT CHAIN; CHAIN: A, C; 7C8 FAB FRAGMENT; LONG CHAIN; CHAIN: B. D | FIBROBLAST GROWTH FACTOR 2; CHAIN: A, B; FIBROBLAST GROWTH FACTOR RECEPTOR 1; CHAIN: C, D; | FIBROBLAST GROWTH FACTOR 2; CHAIN: A, B; FIBROBLAST GROWTH FACTOR RECEPTOR 1; CHAIN: C, D; | FIBROBLAST GROWTH FACTOR 2: CHAIN: A, B; FIBROBLAST GROWTH FACTOR RECEPTOR 1; CHAIN: C, D; | NEURAL CELL ADHESION MOLECULE; CHAIN: A, B, C, D; |
| SeqFold | | · | | | | | | | |
| PMF | | 0.39 | -0.11 | 0 | -0.15 | -1,41 | 0.43 | 0.34 | 0.99 |
| Verify score | | 0.25 | 60'0 | 90.0 | 0.11 | 0.1 | 0.18 | 1.0 | 0.16 |
| PSI- BLAST | | 7.00E-20 | 1.40E-48 | 1.40E-50 | 6.80E-13 | 1.40E-44 | 3.40E-28 | 1.40E-30 | 5.60E-30 |
| End | | 435 | 522 | 436 | 328 | 340 | 225 | 220 | 214 |
| Start | | 252 | 137 | 32 | 140 | 134 | 31 | 36 | 33 |
| Chain ID | | | ٧ | A | ¥ | ပ | Д | Δ | ∢ |
| PDB DD | | 1cfb | 1cs6 | les6 | lct8 | lcvs | Icvs | lcvs | lepf |
| SEQ NO D | | 578 | 578 | 878 | 578 | 578 | 578 | 578 | 878 |

| PDB annotation | GROWTH FACTOR/GROWTH FACTOR RECEPTOR FGPS, FGRRZ, IMAUNOGLOBULIN (IGILIKE DOMANNS BELONGING TO THE I-SET 2 SUBGROUP WITHIN IG-LIKE DOMANNS, B-TREFOLI FOLD | GROWTH FACTOR/GROWTH FACTOR REGEPTOR FGP2; FGFR2; IMMUNOGLOBULIN (19LIKE DOMANNS BELONGING TO THE I-SET 2 SUBGROUP WITHIN 10-LIKE DOMANNS, B-TREFOLI FOLD | GROWTH FACTOR/GROWTH FACTOR RECEPTOR FGF1; FGFR1; INAUTORICABULIN (1G) LIKE DOMANNS BELONGING TO THE I-SET 3 SUBGROUP WITHIN 1G-LIKE DOMANINS, B-TREFOLI FOLD | HORMONEGROWTH FACTORHORMONE RECEPTOR 4- HELICAL BUNDLE, ALPHA HELICAL BUNDLE, TERNARY COMPLEX, FN 2 BUNDLE, TERNARY SHEET DOMARNS, CYTOKINE-RECEPTOR COMPLEX CYTOKINE-RECEPTOR COMPLEX | CONTRACTILE PROTEIN IMMUNOGLOBULIN FOLD, BETA BARREL | CELL ADHESION PROTEIN RGD, EXTRACELLULAR MATRIX 1FNF 18 | HEPARIN AND INTEGRIN BINDING HEPARIN AND INTEGRIN BINDING | | | | IMMUNOGLOBULIN INTACT |
|------------------|--|--|---|--|--|---|--|---|---|---|-----------------------|
| Coumpound | FIBROBLAST GROWTH FACTOR 2; CHAIN: A, B, C, D; FIBROBLAST GROWTH FACTOR RECEPTOR 2; CHAIN: E, F, G, H; | FIBROBLAST GROWTH FACTOR 2; CHAIN: A, B, C, D; FIBROBLAST GROWTH FACTOR RECEPTOR 2; CHAIN: E, F, G, H; | FIBROBLAST GROWTH FACTOR I; CHAIN: A, B; FIBROBLAST GROWTH FACTOR RECEPTOR I; CHAIN: C, D; | PLACENTAL LACTOGEN; CHAIN: A; PROLACTIN RECEPTOR: CHAIN: B, C; | TELOKIN; CHAIN: A | FIBRONECTIN; IFNF 6 CHAIN: NULL; IFNF 7 | FIBRONECTIN; CHAIN: A; | T LYMPHOCYTE ADHESION GLYCOPROTEIN CD2 (HUMAN) 1HNF 3 | T LYMPHOCYTE ADHESION GLYCOPROTEIN CD2 (RAT) IHNG 3 | T LYMPHOCYTE ADHESION GLYCOPROTEIN CD2 (RAT) IHNG 3 | IGGI INTACT ANTIBODY |
| SeqFold | | | | | | | | | | | 95.64 |
| PMF | 0.25 | 0.48 | 0.01 | 0.17 | -0.05 | 0.46 | 9.04 | 0.29 | -0.12 | 0.15 | |
| Verify score | 60.0 | 90.0- | 0.03 | 0.29 | 0.06 | 0.24 | 0.24 | 0.3 | 0.05 | 0.15 | |
| PSI. BLAST | 4.20E-30 | 2.80E-31 | 5.60E-28 | 1.40E-11 | 6.80E-18 | S.60E-15 | 1.40E-12 | 1.40E-18 | 4.20E-14 | 2.80E-24 | 3.40E-10 |
| End | 220 | 228 | | 436 | 131 | 432 | 432 | 211 | 292 | 727 | 454 |
| Start | 38 | 36 | | 267 | 27 | 264 | 264 | 47 | 143 | 49 | 34 |
| Chain | ωl | O | ပ | ω | ⋖ | | ٧ | | ∢ | ¥ | В |
| PDB ED | lev2 | lev2 | levt | 1f6f | 1fhg | 1faf | ųIJĮ. | Ihnf | lhng | lhng | 578 ligy |
| SEQ No en SEQ | 878 | 878 | 578 | 578 | 578 | 878 | 878 | 578 | 578 | 578 | 278 |

| | , | · · | | | | | | |
|------------------|---|--|--|---|---|---|--|---|
| PDB annotation | IMMUNOGLOBULIN, V REGION, C REGION, HINGE REGION | COMPLEX (IMAMUNOGLOBULINRECEPTOR) IMANINOGLOBULINREDLD, TRANSMENGRANE, GLYCOPROTEIN, RECEPTOR, 2 SIGNAL, COMPLEX (IMANINOGLOBULINRECEPTOR) | - | CELL ADHESION PROTEIN CELL ADHESION PROTEIN, RGD, EXTRACELLULAR MATRIX, 2 HEPARIN-BINDING, GLYCOPROTEIN | MUSCLE PROTEIN CONNECTIN, NEXTMS, CELL ADHESION, GLYCOPROTEIN, TRANSMEMBRANE, REPEAT, BRAIN, 2 IMATINOGLOBULIN FOLD, ALTERNATITY SERJOING, SIGNAL, 3 ALTERNATITY SERJOING, SIGNAL, 3 AMINCY PROTEIN | MUSCLE PROTEIN CONNECTIN, NEXTAS, CELL ADHESION, GLYCOPROTEIN, TRANSMEMBRANE, REPEAT, BRAIN, 2 DAMINOGLOBULIN FOLD, ALTERNATITY SEPICING, SIGNAL, 3 AMISCLE PROTEIN | MUSCLE PROTEIN CONNECTIN, NEXTMS; CELL ADHESION, GLYCOPROTEIN, TRANSMEMBRANE, REPEAT, BRAIN, 2 IMMUNOCLOBULIN FOLD, ALTERNATIVE SPLICING, SIGNAL, 3 ALTERNATIVE SPLICING, SIGNAL, 3 MUSCLE PROTEIN | STRUCTURAL PROTEIN INTEGRIN, HEMIDESMOSOME, FIBRONECTIN, CARCINOMA, STRUCTURAL 2 PROTEIN |
| Coumpound | MAB61.1.3; CHAIN: A, B, C, D | INTERLEUKIN-1 BETA; CIAADI. A; TYPE 1 INTERLEUKIN-1 RECEPTOR; CHAIN: B; | IMMUNOGLOBULIN IMMUNOGLOBULIN GI (IGGI) (MCG) WITH A HINGE DELETION IMCO 3 | FIBRONECTIN; CHAIN: NULL; | TITIN, CHAIN: NULL; | TITIN; CHAIN: NULL; | TITIN; CHAIN: NULL; | INTEGRIN BETA-4 SUBUNIT; CHAIN: A, B; |
| SeqFold score | | · | 96.36 | | | | | |
| PMF | | -0.12 | | 0.33 | 0.88 | 90.0- | -0.13 | 0.52 |
| Verify score | | 0.03 | | 0.39 | 0.29 | 90.00 | 0.13 | 0.3 |
| PSI- BLAST | | 6.80E-34 | 3.40E-10 | 1.30E-17 | 1.40E-18 | 4.20E-15 | 6.80E-15 | 1.40E-20 |
| End | | 338 | 423 | 432 | 227 | 132 | 132 | 450 |
| Start AA | | 25 | 32 | 264 | | 31 | 31 | 251 |
| Chain ID | | В | н | | | | | ¥ |
| PDB DD | | lifib | o o | 1mfn | Inct | lnct | Inct | lqg3 |
| SEQ B SEQ | | 578 | 578 | 578 | 578 | 578 | 578 | 578 |

| PDB annotation | STRUCTURAL PROTEIN TENASCIN, FIBRONECTIN TYPE-III, HEPARIN, EXTRACELLULAR 2 MATRIX, ADHESION, FUSION PROTEIN, STRUCTURAL PROTEIN | | | | GLYCOPROTEIN CD4; IMMUNOCLOBULIN FOLD, TRANSMEMBRANE, GLYCOPROTEIN, T-CELL, 2 MHC LIPOPROTEIN, POLYMORPHISM | MUSCLE PROTEIN IMMUNOGLOBULIN SUPERFAMILY, I SET, MUSCLE PROTEIN | MUSCLE PROTEIN IMMUNOGLOBULIN SUPERFAMILY, I SET, MUSCLE PROTEIN | NERVE GROWTH FACTORTRKA COMPLEX, BETA-MET, COMPLEX, TRKA RECEPTOR, NERVE GROWTH FACTOR, CY STEINE KNOT, 2 IMMUNOCLOBULIN LIKE DOMAIN, NERVE GROWTH FACTORTRKA | CELL ADHESION ICAM-2; IMMUNOGLOBULIN FOLD, CELL ADHESION, GLYCOPROTEIN, 2 TRANSMEMBRANE, REPEAT, SIGNAL |
|------------------|--|--|--|---|---|--|--|---|--|
| Coumpound | TENASCIN; CHAIN: A, B; | MUSCLE PROTEIN TITIN MODULE MS (CONNECTIN) ITINM 3 (WMR, MINIMIZED AVERAGE STRUCTURE) ITINM 4 ITINM 38 | MUSCLE PROTEIN TITIN MODULE MS (CONNECTIN) ITINM 3 (NMR, MINIMIZED AVERAGE STRUCTURE) ITINM 4 ITINM 38 | GLYCOPROTEIN FIBRONECTIN (TENTH TYPE III MODULE) (NMR, 36 STRUCTURES) ITTF 3 | T-CELL SURFACE GLYCOPROTEIN CD4; CHAIN: A, B; | TWITCHIN 18TH IGSF MODULE; CHAIN: NULL; | TWITCHIN 18TH 1GSF MODULE; CHAIN: NULL; | NERVE GROWTH FACTOR; CHAIN: Y, W; TRKA RECEPTOR; CHAIN: X, Y; | INTERCELLULAR ADHESION MOLECULE-2; CHAIN: NULL; |
| SeqFold score | | | | | | | | | |
| PMF | 0.82 | 68.0 | 0.03 | 0.05 | -0.12 | 0.78 | 0.1 | -0.01 | 0.23 |
| Verify score | 0.52 | 0.39 | -0.04 | 0.2 | 0.04 | 0.52 | 0.23 | 0.02 | 0.18 |
| PSI- BLAST | 2.80E-17 | 7.00E-18 | 8.40E-15 | 1.40E-10 | 2.80E-20 | 2.80E-17 | 2.80E-15 | 5.60E-18 | 1.10E-30 |
| End | 435 | 727 | 132 | 434 | 281 | 226 | 132 | 228 | 228 |
| Start | 264 | 139 | | 346 | | 139 | 31 | 142 | 31 |
| Chain | ∢ | | | | < | | | × | |
| PDB CD | 1914 | Ifm | Itnm | Ħ | Iwio | lwit | Iwit | ww w | bzzl |
| SEQ No. | 578 | 578 | 578 | 578 | 578 | 578 | 578 | 578 | 578 |

| | | , | | | | | | , | |
|------------------|---|---|--|--|--|--|---|---|---|
| PDB annotation | IMMUNE SYSTEM PS8 NATURAL KILLER CELL RECEPTOR; KIR, NATURAL KILLER RECEPTOR, NATURAL KILLER RECEPTOR, IMMUNOGLOBULIN | IMMUNE SYSTEM CD32; RECEPTOR, FC, CD32, IMMUNE SYSTEM | PROTEIN BINDING ED-B, FIBRONECTIN, TYPEIII DOMAIN, ANGIOGENESIS, PROTEIN 2 BINDING | COAGULATION FACTOR | CELL ADHESION NCAM DOMAIN 1; CELL ADHESION, GLYCOPROTEIN, HEPARIN-BINDING, GPI-ANCHOR, 2 NEURAL ADHESION MOLECULE, IMMUNOGI.OBIUJIN, FOILD, SIGNAL | | CELL ADHESION PROTEIN NCAM MODILE 2; CELL ADHESION, MODILE 2; CELL ADHESION, CELL COLL CHARLA BINDING, GP-ANCHOR, 2 NEURAL ADHESION MOLECULE, IMMUNOGLOBULIN FOLD, HOMOPHILC 3 BINDING, CELL ADHESION PROTEIN | CELL ADHESION PROTEIN NCAM MODILE 2; CELL ADHESION, MODILE 2; CELL ADHESION, CELVCORKOTEN; HEPARN-BINDING, GPI-ANCHOR, 2 NEURAL ADHESION MOLECULE, IBMAUDOBLOBULIN POLL), HOMOPHILIG 3 BINDING, CELL ADHESION PROTEIN | |
| Coumpound | MHC CLASS I NK CELL RECEPTOR PRECURSOR; CHAIN: A; | FC GAMMA RIB; CHAIN: A; | FIBRONECTIN, CHAIN: A; | HUMAN TISSUE FACTOR; 2HFT 4 CHAIN: NULL; 2HFT 5 | NEURAL CELL ADHESION MOLECULE; CHAIN: NULL; | HORMONE/RECEPTOR HUMAN GROWTH HORMONE COMPLEXED WITH ITS RECEPTOR 3HHR 3 EXTRACEL/ULAR DOMAIN 3HHR 4 | NEURAL CELL ADHESION MOLECULE, LARGE ISOFORM; CHAIN: A; | NEURAL CELL ADHESION MOLECULE, LARGE ISOFORM; CHAIN: A; | VIRUS EQUINE HERPES VIRUS-1 (C3HC4, OR RING |
| SeqFold score | | | | | | | | | |
| PMF | -0.02 | 99.0 | -0.12 | 90.0 | 0.98 | -0.09 | 0.31 | 90:0 | 0.01 |
| Verify score | 0.25 | 0.1 | 0.45 | 0.13 | 0.64 | 0.06 | 0.06 | 0.04 | -0.56 |
| PSI- BLAST | 2.80E-25 | 2.80E-33 | 1.40E-12 | 2.80E-12 | 5.60E-18 | 5.60E-17 | 4.20E-18 | 7.00E-17 | 1.00E-09 |
| End | 220 | 228 | 435 | 436 | 227 | 436 | 220 | 134 | 103 |
| Start | 30 | 31 | 343 | 264 | 139 | | 139 | 32 | 19 |
| Chain ID | ¥ | V | Ą | | | В | ¥ | ٧ | |
| PDB CD | 2dli | 2fcb | 2fnb | 2hft | Znc m | 3hhr | 3nc m | 3nc m | 1chc |
| S e S | 578 | 578 | 578 | 278 | 278 | 578 | 578 | 578 | 579 |

| PDB annotation | | TRANSCRIPTION FACTOR BTF2 P44 SUBUNIT; BASIC TRANSCRIPTION FACTOR, ZINC BINDING PROTEIN | DNA-BINDING PROTEIN V(D)J | RECOMBINATION ACTIVATING | PROTEIN 1; RAG1, V(D)J | RECOMBINATION, ANTIBODY, MAD, | RING FINGER, 2 ZINC BINUCLEAR | CLUSTER, ZINC FINGER, DNA- | BINDING PROTEIN | DNA-BINDING PROTEIN V(D)J | RECOMBINATION ACTIVATING | PROTEIN 1; RAG1, V(D)J | RECOMBINATION ANTIBODY MAD | PRICERICED 12NO PRINCIPAD | KING FINGER, 2 ZINC BINOCLEAR | CLUSTER, ZINC FINGER, DNA- | BINDING PROTEIN | DNA-BINDING PROTEIN V(D)J | RECOMBINATION ACTIVATING | PROTEIN 1; RAG1, V(D)J | RECOMBINATION, ANTIBODY, MAD. | RING FINGER, 2 ZINC BINUCLEAR | CLUSTER, ZINC FINGER, DNA- | BINDING PROTEIN | CALCIUM-BINDING PROTEIN CALB; | CALCIUM++/PHOSPHOLIPID BINDING | PROTEIN, 2 CALCIUM-BINDING | BADOCYTOSIS/EVOCATOSIS | SALAMOTT CHISTOCK TOSIS | STINATIOI AUMIN, CA-DOMAIN, | THE PAST | 2 KELEASE, FNDOCYTOSIS/FXOCYTOSIS | HYDROLASE CPLA2: | PHOSPHOI IPASE 1 IPID. BINDING | HYDROLASE | TRANSFERASE CALCIUM++. | PHOSPHOLIPID BINDING PROTEIN, CALCIUM-BINDING 2 PROTEIN, |
|-----------------|------------------|---|---------------------------|--------------------------|------------------------|-------------------------------|-------------------------------|----------------------------|-----------------|---------------------------|--------------------------|------------------------|----------------------------|---------------------------|-------------------------------|----------------------------|-----------------|---------------------------|--------------------------|------------------------|-------------------------------|-------------------------------|----------------------------|-----------------|-------------------------------|--------------------------------|----------------------------|--------------------------|---------------------------|-----------------------------|----------|--------------------------------------|------------------|--------------------------------|-----------|-------------------------|--|
| Coumpound | STRUCTURE) ICHC4 | TFIIH P44 SUBUNIT; CHAIN: A; | RAGI; CHAIN: NULL; | | | | | | | RAG1; CHAIN: NULL; | | | | | | | | RAG1; CHAIN: NULL; | | | | | | | PROTEIN KINASE C (BETA); | CHAIN: A, B; | | CVNABTOTACIANI I. CHAIN: | STINATIOI AUMIN I, CHAIN. | ÷ | | | CYTOSOLIC | PHOSPHOLIPASE A2: CHAIN: | A.B. | PROTEIN KINASE C. ALPHA | TYPE; CHAIN: A; |
| SegFold | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.19 | 0.33 | | | | | | | 0.29 | | | | | | | | 0.13 | | | | | | | 0.94 | | | 630 | 70.0 | | | | 0.13 | : | | 86.0 | |
| Verify score | | 0 | 0.0 | | | | | | | -0.78 | | | | | | | | 0.01 | | | | | | | 0.83 | | | 900 | 9.0 | | _ | | 0.05 | | | 0.61 | |
| PSI- BLAST | | 0.00051 | 0.0037 | | | | | | | 0.0007 | | | | | | | | 3.40E-07 | | | | | | | 1.70E-30 | | | 1 705 23 | 1./05-23 | | | | 1.70E-15 | ? | | 3.40E-31 | |
| End | | 102 | 268 | | | | | | | 35 | | | | | | | | 128 | | | | | | | 1443 | | | CVVI | 74 | | | | 1444 | | | 1443 | |
| Start AA | | 21 | 223 | | | | | | | 29 | | | | | | | | 63 | | | | | | | 1329 | | | 1335 | 77 | | | • | 1342 | ! | | 1329 | |
| Chain ID | | ¥ | | | | | | | | | | | | | | | | | | | | | | | A | | | 4 | c | | | | V | : | | Ą | |
| PDB CD | | 1.00 E+53 | 1rmd | | | | | | | Irmd | | | | | | | | 1rmd | | | | | | | 1a25 | | | 1 hvm | ıı karı | | | | 1civ | 3 | | 1dsy | |
| SEQ B B SE | | 579 | 579 | | | | | | | 579 | | | | | | | | 579 | | | | | | | 280 | | | 580 | 8 | | | | 280 | | | 280 | |

| PDB annotation | PHOSPHATIDYLSERINE, PROTEIN KINASE C | PHOSPHOINOSITIDE 3-KINASE GAMMA PTDINS-3-KINASE P110, PI3K, P1 3K; PHOSPHOINOSITIDE 3-KINASE GAMMA, SECONDARY MESSENGER 2 | GENERATION, PI3K, PI 3K, WORTMANNIN | PHOSPHOINOSITIDE 3-KINASE GAMMA PTDINS-3-KINASE P110, P13K; PHOSPHOINOSITIDE 3-KINASE GAMMA, SECONDARY MESSENGER 2 GENERATION, P13K, P1 3K | HYDROLASE CALB DOMAIN; HYDROLASE, C2 DOMAIN, CALB DOMAIN | | ENDOCYTOSIS/EXOCYTOSIS C2- DOMAINS, C2B-DOMAIN, RABPHILIN, ENDOCYTOSIS/EXOCYTOSIS | SIGNALING PROTEIN GUANINE NUCLEDTINE BINDING PROTEIN 1; GBP, GTP HYDROLYSIS, GDP, GMP, INTERFERON INDUCED, DYNAMIN 2 RELATED, LARGE CIPASE FAMILY, SIGNALING PROTEIN | SIGNALING PROTEIN GBP, GTP HYDROLYSIS, GDP, GMP, INTERERON INDUCED, DYNAMIN 2 RELATED, LARGE GTPASE FAMILY, GMPPNP, GPPNHP. | PHOSPHOTRANSFERASE | PHOSPHOGLUCOMUTASE; 3PMG 6 PHOSPHOGLUCOMUTASE 3PMG 13 | PHOSPHOTRANSFERASE PHOSPHOGLUCOMUTASE; 3PMG 6 |
|------------------|---|--|-------------------------------------|--|--|---|---|--|---|----------------------|---|--|
| Coumpound | | PHOSPHATIDYLINOSITOL 3- KINASE CATALYTIC SUBUNIT; CHAIN: A; | | PHOSPHATIDYLNOSITOL 3 KINASE CATALYTIC SUBUNIT; CHAIN: A; | PHOSPHOLIPASE A2; CHAIN: NULL; | CALCIUM/PHOSPHOLIPID BINDING PROTEIN SYNAPTOTAGMIN I (FIRST C2 DOMAIN) (CALB) IRSY 3 | RABPHILIN 3-A; CHAIN: A; | INTERFERON-INDÚCED GUANYLATE-BINDING PROTEIN I; CHAIN: A; | INTERFERON-INDUCED GUANYLATE-BINDING PROTEIN I; CHAIN: A; | ALPHA-D-GLUCOSE-1,6- | BISPHOSPHATE; 3PMG 4 CHAIN: A, B; 3PMG 5 | ALPHA-D-GLUCOSE-1,6- BISPHOSPHATE; 3PMG 4 |
| SeqFold | | | | - | | | | | | | | 129.26 |
| PMF | | 1202.08 | | -1.41 | 0.64 | 0.59 | 0.39 | -0.2 | -0.2 | -0.2 | | |
| Verify score | | 0.15 | | 0.15 | -0.02 | 90:0 | 0.1 | 0.27 | 0.47 | 0.29 | | |
| PSI- BLAST | | 0 | | 0 | 1.70E-15 | 8.50E-24 | 5.10E-29 | 0 | 0 | 0 | | 0 |
| End AA | | 1175 | | 1175 | 1444 | 1442 | 1441 | 21.5 | 27.5 | 604 | | 119 |
| Start AA | | 214 | | 297 | 1342 | 1321 | 1328 | 9 | 7 | 46 | | S |
| Chain ID | | ∢ . | | ٧ | | | ٧ | ∢ | ∢ | ¥ | | ∢ |
| PDB ID | | le7u | | le8y | Iriw | Irsy | Зтрь | 14g3 | 15n | 3pm | 600 | 3pm g |
| SEQ ID NO: | | 280 | | 280 | 280 | 280 | 280 | 285 | 285 | 286 | | 286 |

| | | | | | | -: | | | | | |
|------------------|----------------------------|--|--|---|--|---|---|--|--|---|--|
| PDB annotation | PHOSPHOGLUCOMUTASE 3PMG 13 | TRANSCRIPTION REGULATION PROTO-ONCOGENE, NUCLEAR BODIES (PODS), LEUKEMIA, 2 TRANSCRIPTION REGULATION | TRANSCRIPTION REGULATION PROTO-ONCOGENE, NUCLEAR BODIES (PODS), LEUKEMÍA, 2 TRANSCRIPTION REGULATION | | LIGASE CBL, UBCH7, ZAP-70, E2, UBIQUITIN, E3, PHOSPHORYLATION, 2 TYROSINE KINASE, UBIQUITINATION, PROTEIN DEGRADATION, | METAL BINDING PROTEIN RING FINGER PROTEIN MAT1; RING FINGER (C3HC4) | METAL BINDING PROTEIN RING FINGER PROTEIN MATI; RING FINGER (C3HC4) | LIM DOMAIN CONTAINING PROTEINS LIM DOMAIN CONTAINING PROTEINS, METAL-BINDING PROTEIN, ZINC 2 FINGER | LIM DOMAIN CONTAINING PROTEINS LIM DOMAIN CONTAINING PROTEINS, METAL-BINDING PROTEIN, ZINC 2 FINGER | CONTRACTILE LIM DOMAIN, CRP, NMR, MUSCLE DIFFERENTIATION, CONTRACTILE | METAL-BINDING PROTEIN LIM DOMAIN CONTAINING PROTEINS ICTL 15 |
| Coumpound | CHAIN: A, B, 3PMG 5 | TRANSCRIPTION FACTOR PML; CHAIN: NULL; | TRANSCRIPTION FACTOR PML; CHAIN: NULL; | VIRUS EQUINE HERPES VIRUS-1 (C3HC4, OR RING DOMAIN) ICHC 3 (NMR, 1 STRUCTURE) ICHC 4 | SIGNAL TRANSDUCTION PROTEIN CBL. CHAIN: A: ZAP-70 PEPTIDE: CHAIN: B; UBIQUITIN-CONJUGATING ENZYME E12-18 KDA UBCH7; CHAIN: C; | CDK-ACTIVATING KINASE ASSEMBLY FACTOR MATI; CHAIN: A; | CDK-ACTIVATING KINASE ASSEMBLY FACTOR MAT1; CHAIN: A; | QCRP2 (LIM1); CHAIN: NULL; | QCRP2 (LIMI); CHAIN: NULL; | CRPI; CHAIN: A; | AVIAN CYSTEINE RICH PROTEIN; ICTL 3 |
| SeqFold score | | | | | | | | | | | |
| PMF | | 0.25 | 0.11 | 86.0 | 6:0 | 0.48 | 60.0 | 0.62 | 0 | 0.18 | 0.16 |
| Verify | | -0.73 | -0.62 | 0.24 | 0.25 | 0.19 | -0.44 | -0.16 | .0· | -0.11 | -0.11 |
| PSI- BLAST | | 8.50E-06 | 8.40E-08 | 8.50E-15 | 1.70E-10 | 8.40E-08 | 1.20E-05 | 9.80E-17 | 1.40E-11 | 4.20E-11 | 1.10E-12 |
| End | | 65 | <u>۶</u> . | 09 | 99 | 2 | 72 | 592 | 995 | 629 | 629 |
| Start | | 16 | | 91 | 81 | 17 | 81 | 536 | 297 | 297 | 969 |
| Chain | | | | | | ٧ | 4 | | | ⋖ | |
| 80. 10 | | Ibor | 1bor | Ichc | 1fbv | 1g25 | 1825 | la7i | la7i | 158t | 1ct |
| S a S | | 587 | 587 | 587 | 587 | 587 | 587 | 592 | 292 | 292 | 292 |

| PDB annotation | SIGNALING PROTEIN LIM DOMAIN CONTAINING PROTEINS, METAL- BINDING PROTEIN | SIGNALING PROTEIN LIM DOMAIN CONTAINING PROTEINS, METAL- BINDING PROTEIN | METAL-BINDING PROTEIN CRIP; METAL-BINDING PROTEIN, LIM DOMAIN PROTEIN | METAL-BINDING PROTEIN CRIP; METAL-BINDING PROTEIN, LIM DOMAIN PROTEIN | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | ANTI-ONCOGENE CELL CYCLE, ANTI- ONCOGENE, REPEAT, ANK REPEAT | COMPLEX (TRANSCRIPTION REGULATION/DNA) GABPALPHA; | GABPBETAI; COMPLEX (TRANSCRIPTION | REGULATION/DNA), DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, | ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, | COMPLEX (KINASE/ANTI- | ONCOGENE) CDK6; P16INK4A, MTS1; CYCLIN DEPENDENT KINASE | CYCLIN DEPENDENT KINASE | INHIBITORY 2 PROTEIN, CDK, INK4, | CELL CYCLE, MULTIPLE TUMOR SUPPRESSOR, 3 MTSL COMPLEX | (KINASE/ANTI-ONCOGENE) HEADER | COMPLEX (INHIBITOR PROTEIN/KINASE) INHIBITOR |
|------------------|--|--|---|---|--|---|---|--|---|--|---|-----------------------|--|-------------------------|----------------------------------|--|-------------------------------|---|
| Coumpound | CYSTEINE AND GLYCINE- RICH PROTEIN CRP2; CHAIN: A; | CYSTEINE AND GLYCINE- RICH PROTEIN CRP2; CHAIN: A; | CYSTEINE RICH INTESTINAL PROTEIN; CHAIN; NULL; | CYSTEINE RICH INTESTINAL PROTEIN; CHAIN; NULL; | DNA, CHAIN: A, B, D, E, CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G, | TUMOR SUPPRESSOR PIGINK4A; CHAIN: NULL: | GA BINDING PROTEIN ALPHA; CHAIN: A; GA | BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; | | | P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | CYCLIN-DEPENDENT | KINASE 6; CHAIN: A; MULTIPLE TUMOR | SUPPRESSOR; CHAIN: B; | | | | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; |
| SeqFold score | | | | | | | | | | | | | | | | | | |
| PMF | 8.0 | 0.23 | 0.29 | 0.07 | -0.19 | 0.72 | 0.1 | | | | 97.0 | 0.82 | | | | | | 0.84 |
| Verify | 0.43 | -0.27 | -0.42 | 0.15 | 0.16 | 0.1 | 0.35 | | | | 0.28 | 0.02 | | | | | | 0.23 |
| PSI- BLAST | 1.40E-16 | 1.10E-13 | 1.30E-19 | 4.20E-13 | 1.20E-10 | 0.00014 | 0.00014 | - | | | 0.00011 | 9.80E-05 | | | | | | 0.00011 |
| End | 592 | 199 | 609 | 699 | 395 | 370 | 369 | | | | 370 | 367 | | | | | | 367 |
| Start AA | 535 | 292 | 537 | 296 | 367 | 315 | 315 | | | | 315 | 315 | | | | | | 315 |
| Chain ID | ¥ | ٧ | | | ဗ | | В | | | | | m | | | | | | В |
| PDB ID | 1cxx | lexx | liiil | liml | Jme y | laSe | lawc | | | | 1bd8 | 1bi7 | | | | | | 1blx |
| SEQ NO DE | 592 | 592 | 592 | 592 | 592 | 293 | 293 | | | | 593 | 593 | | | | | | 293 |

| PDB annotation | PROTEIN, CYCLIN-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHA/BETA, COMPLEX (INHIBITOR PROTEIN/KINASE) | COMPLEX (INHIBITOR POPULAR AND | SIGNALING PROTEIN HELIX-TURN- HELIX, ANKYRIN REPEAT | METAL BINDING PROTEIN ZINC- BINDING MODULE, ANKYRIN REPEATS, METAL, BINDING PROTEIN | TRANSCRIPTION FACTOR P65, P50D; TRANSCRIPTION FACTOR, IKB/NFKB COMPLEX | COMPLEX (TRANSCRIPTION REGIANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX | KINASE KINASE, SIGNAL TRANSDUCTION, CALCIUM/CALMODULIN | |
|----------------|---|--|--|---|--|---|--|--|
| Coumpound | P19INK4D; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B; | CYCLIN-DEPENDENT KINASE 4 INHIBITOR B; CHAIN: A; | PYK2-ASSOCIATED PROTEIN BETA; CHAIN: A; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-AI,PHA: CHAIN: D: | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E, F; | CALCIUM/CALMODULIN- DEPENDENT PROTEIN KINASE: CHAIN: NULL: | TRANSFERASE/PHOSPHOTR ANSFERASE) SC-AMPS- DEPONDENT PROTEIN KINASE (CLZ.1.137) (SCAPKS) IAPM 3 LPHA ISOENZYME MUTANT WITH SER 139 LAPM A REPACED BY ALA (S19AS) COMPLEX WITH THE PETTIDE IAPM 5 IHE PETTIDE IAPM 5 IHE DETTEGEN WEGA-8 |
| SeqFold | | | | | | | | |
| PMF | | 0.76 | 0.21 | 0.76 | 0.98 | 0.59 | | - |
| Verify | | 0.42 | -0.02 | 0.4 | 0.31 | 0.25 | 0.15 | 0.23 |
| PSI- BLAST | | 0.00011 | 1.40E-05 | 8.40E-05 | 0.00014 | 2.80E-06 | 5.10E-90 | 0 |
| End | | 370 | 370 | 370 | 370 | 381 | 302 | 318 |
| Start AA | | 315 | 315 | 315 | 315 | 315 | 61 | 25 |
| Chain 10 | | ш | ٧ | ¥ | D | Э | | ш |
| PDB ID | | 19lx | 149s | 1deq | lika | lufi | 1a06 | lap m |
| SEQ NO ID | | 593 | 593 | 593 | 593 | 593 | 594 | |

| PDB annotation | | - | PROTEIN KINASE CDK2; PROTEIN KINASE, CELL CYCLE, PHOSPHORYLATION, STAUROSPORINE, CELL DIVISION, MITOSIS, INHIBITION | COMPLEX (INHIBITOR PROTEIN/KINASE) INHIBITOR PROTEIN, CYCLIA-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHADELT, COMPLEX (INHIBITOR PROTEIN/KINASE) | | | |
|-----------------|--------|---|---|---|---|---|---|
| Conmpound | 1APM 6 | TRANSTERASE PHOSPHOTA ANSTERASE SCAMPS- DEPENDENT PROTEIN KINAGE (E.C.2.7.1.37) (SCIARKS) IAPM 3 (CATALYTE SUBGINIT) ALHAI SOBNIZIME MUTANT WITH SER 119 IAPM 4 REPLACED BY ALA (RS19AS) COMPLEX WITH THE PERTIDE IAPM 3 INHIBITOR RK(5.24) AND THE DESTIDE IAPM 3 INHIBITOR PK(4.24) AND THE DESTIDE IAPM 3 INHIBITOR PK(4.24) AND THE DESTIDENT IAPM 3 INHIBITOR PK(4.24) AND THE DESTIDENT IAPM 3 INHIBITOR PK(4.24) AND THE DESTINATION AND THE | CYCLIN-DEPENDENT PROTEIN KINASE 2; CHAIN: NULL; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B; | PHOSPHOTRANSFERASE CAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT ICMK 3 (E.C.2.7.1.37) ICMK 4 | PHOSPHOTRANSFERASE CAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT ICMK 3 (E.C.2.7.1.37) ICMK 4 | TRANSFERASE(PHOSPHOTR ANSFERASE) CAMP- DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (CAPK) ICTP 3 (CATALYTIC |
| SeqFold | | 125.65 | 120.88 | 127.11 | 127.4 | | 127.61 |
| PMF | | | | | | _ | |
| Verify score | | | | | | 0.33 | |
| PSI- BLAST | | 0 | 1.40E-60 | 7.00E-56 | 0 | 0 | 0 |
| End | | 325 | 308 | 325 | 328 | 318 | 328 |
| Start AA: | | 'n | | 22 | | 25 | 2 |
| Chain D | | ш | | ¥ | 1 | ല | п |
| PDB ID | | en e | laqı | 1blx | lcm k | lcm k | Ictp |
| SEQ B B SE | | 594 | 594 | 594 | 594 | 594 | 594 |

| | 1 | | | | | | | | | | _ | | | | _ | | | |
|------------------|--|--|-----------------|--|--|---|--|--|--|---|----------------------------|---|-------------------------------|------------------------------|----------------------------|--|-------------------------------|-----------------------------|
| PDB annotation | The state of the s | | | ENDOCYTOSIS/EXOCYTOSIS NSECI; PROTEIN-PROTEIN COMPLEX, MULTI-SUBUNIT | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGMIN ASSOCIATED 35 KDA PROTEIN, P35A, THREE HELIX BUNDLE | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGMIN ASSOCIATED 35 | KUA PROTEIN, P35A, THREE HELIX BUNDLE | TRANSFERASE KINASE DOMAIN, AUTOINHIBITORY FRAGMENT, | НОМОВІМЕК | TRAÑSFERASE KINASE DOMAIN, AUTOINHIBITORY FRAGMENT, HOMODIMER | PHOSPHOTRANSFERASE FGFRIK, | FIBROBLAST GROWTH FACTOR RECEPTOR 1-TRANSFERASE | TYROSINE-PROTEIN KINASE, ATP- | RECEPTOR, PHOSPHOTRANSFERASE | PHOSPHOTRANSFERASE FGFRIK, | FIBROBLAST GROWTH FACTOR PECEPTOR 1: TRANSEED ASE | TYROSINE-PROTEIN KINASE, ATP- | BINDING, 2 PHOSPHORYLATION. |
| Coumpound | SUBUNIT) ICTP 4 | TRANSFERASE(PHOSPHOTR ANSFERASE) CAMP. DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (CAPK) ICTP 3 (CATAI.YTIC | SUBUNIT) ICTP 4 | SYNTAXIN BINDING PROTEIN 1; CHAIN: A; SYNTAXIN 1A; CHAIN: B; | SYNTAXIN-1A; CHAIN: A, B, C; | SYNTAXIN-1A; CHAIN: A, B, C; | | SERINE/THREONINE- PROTEIN KINASE PAK- | ALPHA; CHAIN: A, B; SERINE/THREONINE- PROTEIN KINASE PAK- A1 PHA: CHAIN: C D: | SERNETHREONINE. PROTEIN KINASE PAK. ALPHA, CHAIN: A, B; SERNETHREONINE. PROTEIN KINASE PAK. | FGF RECEPTOR 1; CHAIN: A, | ží. | | | FGF RECEPTOR 1; CHAIN: A, | ža" | | |
| SeqFold score | | | | | | | | | | | 125.79 | | | | 130.09 | | | |
| PMF score | | 1 | | -0.11 | -0.19 | -0.18 | | - | | 1202.08 | | | | | | | | |
| Verify score | | 0.25 | | 0.06 | 0.1 | 91.0 | | 0.5 | | 0.43 | | | | | | | | |
| PSI- BLAST | | 0 | | 4.20E-12 | 1.40E-08 | 2.80E-09 | | 5.60E-86 | | 1.20E-67 | 5.10E-34 | | | | 1.20E-40 | | | |
| End AA | | 318 | | 009 | 265 | 219 | | 302 | | 300 | 287 | | | | 286 | | | |
| Start AA | | 25 | | 442 | 452 | 486 | | 4 | | 4 | 20 | | | | = | | | |
| Chain D | | м | | В | ∢ | 4 | | U | | ပ | ٧ | | | | В | | | |
| PDB TD | | प री | | 1dn1 | 1623 | lez3 | | 15m | | 115m | 1fgk | | | | 1. 28 | | | |
| SEQ No. | | 594 | | | 294 | 594 | | 594 | | 594 | 594 | | | | 294 | | | |

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|------------------|------------------------------|---|---|--|--|---|--|--|---|--|
| PDB annotation | RECEPTOR, PHOSPHOTRANSFERASE | PROTEIN KINASE CDK2; TRANSFERASE, SERIUEFITHEONINE PROTEIN KINASE, ATP-BINDING, 2 CELL CYCLE, CELL DIVISION, MITOSIS, PHOSPHORYLATION | PROTEIN KINASE CDK2; TRANSFERASE, SERNETHREONINE PROTEIN KINASE, ATP-BINDING, 2 CELL CYCLE, CELL DIVISION, MITOSIS, PHOSPHORYLATION | KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION | KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION | TRANSFERASE MITOGEN ACTIVATED PROTEIN KINASE; TRANSFERASE, MAP KINASE, SERINE/THREONINE-PROTEIN KINASE, 2 P38 | KINASE RABBIT MUSCLE PHOSPHORYLASE KINASE; GLYCOGEN METABOLISM, TRANSEERASE, SERNETHREONINE- PROTEIN, 2 KINASE, HT-BINDING, CALMODULIN-BINDING | KINASE RABBIT MUSCLE PHOSPHORYLASE KINASE; GLYCOGEN METABOLISM, TRANSFERASE, SERINETHEONINE- PROTEIN, STRANSE, THE-BINDING, CALMODULIN-BINDING | TRANSFERASE MITOGEN ACTIVA TRAD RROTEIN KINASE, MAP 2, ERK2; TRANSFERASE, SERNIBFHREDONINE-PROTEIN KINASE, MAP KINASE, 2 ERK2 | KINASE KINASE, SIGNAL TRANSDUCTION, |
| Coumpound | | HUMAN CYCLIN. DBPENDENT KINASE 2; CHAIN: NULL; | HUMAN CYCLIN- DEFENDENT KINASE 2; CHAIN: NULL; | TWITCHIN; CHAIN: NULL; | TWITCHIN; CHAIN: A, B; | MAP KINASE P38; CHAIN: NULL; | PHOSPHORYLASE KINASE; CHAIN: NULL; | PHOSPHORYLASE KINASE; CHAIN: NULL; | EXTRACELLUILAR REGULATED KINASE 2; CHAIN: NULL; | CALCIUM/CALMODULIN- DEPENDENT PROTEIN |
| SeqFold score | | | 137.2 | | | 130.84 | 127.79 | | 122.57 | |
| PMF score | | 1 | | _ | - | | | _ | | 1202.08 |
| Verify score | | 0.48 | | 0.5 | 0.48 | | | 0.53 | | 0 |
| PSI- BLAST | | 6.80E-62 | 6.80E-62 | 3.40E-71 | 1.70E-71 | 1.20E-51 | 6.80E-88 | 6.80E-88 | 8.50E-50 | 1.00E-66 |
| End AA | | 284 | 312 | 285 | 284 | 356 | 285 | 282 | 325 | 438 |
| Start AA | | 25 | 27 | 20 | 20 | 9 | 61 | 24 | 10 | 140 |
| Chain D | | | | | ٧ | | | | | |
| EDB DD | | Ihel | Ihcl | Ikoa | 1kob | 1p38 | Ірћк | 1phk | 3erk | 1a06 |
| SEQ NO. | | 594 | 594 | 294 | 594 | 594 | 594 | 594 | 594 | 969 |

| PDB annotation | TRANSFERASE TRANSFERASE, SERINETHREONINE-PROTEIN KINASE, CASEIN KINASE, 2 SER/THR KINASE | | PROTEIN KINASE CDK2; PROTEIN KINASE, CELL CYCLE, PHOSPHORYLATION, STAUROSPORINE, 2 CELL DIVISION, MITOSIS, INHBITION | COMPLEX (KINASE/INHIBITOR) CDKK, PISTACK, CYCLIN DEPENDENT KINASE, CYCLIN DEPENDENT KINASE, CYCLIN DEPENDENT KINASE, INHIBITORY 2 RROTBLK, CDK, INK4, CELL CYCLE, COMPLEX (KINASE/INHIBITOR) | COMPLEX (INHIBITOR PROTEINCASE) HIBITOR PROTEINCHASE) HIBITOR KINASE, CELL CYCLEJ CONTROL, ALPHAGETT, COMPLEX (INHIBITOR PROTEIN/KINASE) | TRANSFERASE CŚK; PROTEIN KINASE, C-TERMINAL SRC KINASE, PHOSPHORYLATION, 2 STAUROSPORINE, TRANSFERASE | PHOSPHOTRANSFERASE PROTEIN |
|------------------|---|--|--|--|--|--|----------------------------|
| Coumpound | PROTEIN KINASE CK2/ALPHA-SUBUNIT; CHAIN: NULL; | TRANSPERAZEPHOSPHOTR ANGERAZEP SCAMPS- DEFENDENT PROTEIN KINASE (CLZ. J.1.37) (SCARKS) 1ARM 3 AUTANT WHIT SER 139 IAPM 4 REPLACED BY ALA (S199AS) COMPLEX WITH THE PEPTIME LAWL NIBBOTOR REJCASA NIBBOTOR REJCASA AND THE DEPTIME AND THE DEPT | CYCLIN-DEPENDENT PROTEIN KINASE 2; CHAIN: NULL; | CYCLIN-DEPENDENT KINASE G-FANIN: A, C; CYCLIN-DEPENDENT KINASE INHIBITOR; CHAIN: B, D; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B; | C-TERMINAL SRC KINASE; CHAIN: A; | CASEIN KINASE I DELTA; |
| SeqFold score | | | | | | | |
| PMF | 0.22 | 0.49 | 0.76 | 0.05 | 0.3 | 0.46 | 0.34 |
| Verify score | -0.44 | -0.03 | 0.03 | -0.06 | 0.2 | 0.01 | -0.08 |
| PSI- BLAST | 4.20E-07 | 3.405-100 | 8.50E-49 | 8.50E-32 | 1.70E-35 | 3.40E-30 | 5.60E-09 |
| End | 351 | 434 | 399 | 397 | 398 | 344 | 351 |
| Start | 234 | 122 | 146 | 149 | 149 | 146 | 198 |
| Chain ID | | ш | | ∢ | ∢ | < | V |
| EDB CD | la6o | m m | laqi | 1618 | 1bk | 1byg | Ički |
| Se O So d | 969 | 965 | 596 | 296 | 965 | 965 | 969 |

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|------------------|----------------------------|--|---|--|---|---|--|---|---|
| PDB annotation | KINASE ICKI 18 | TRANSFERASE STRESS-ACTIVATED PROTEIN KINASE-3, ERK6, ERK5; P38-GAMMA, GAMMA, PHOSPHORYLATION, MAP KINASE | | | TRANSFERASE KINASE DOMAIN, AUTOINHIBITORY FRAGMENT, HOMODIMER | PHOSPHOTRANSFERASE FGFR1K, FIBROBLAST GROWNH FACTOR RECEPTOR 1; TRANSFERASE, TYROSINE-PROTEIN KINASE, ATP- BINDING, 2 PHOSPHOTRANSFRASE | PHOSPHOTRANSFERASE FGFR IK, PIBROBLAST GROWN HF ACTOR RECEPTOR 1; TRANSFERASE, TYROSINE-PROTEIN KINASE, ATP-BINDING 2 PHOSPHOTR ANYSTATION, RECEPTOR, PHOSPHOTR ANYSTRASE, ARCEPTOR, PHOSPHOTR ANYSTRASE, ARCEPTOR, PHOSPHOTR ANYSTRASE, AND | TRANSFERASE PLSO, C-ABL; KINASE, KINASE INHIBITOR, STI-571, ACTIVATION LOOP | PROTEIN KINASE CDK2; TRANSFERASE, SERINE/THREONINE PROTEIN KINASE, ATP-BINDING, 2 CELL CYCLE, CELL DIVISION, |
| Coumpound | ICKI 6 CHAIN: A, B; ICKI 7 | PHOSPHORYLATED MAP KINASE P38-GAMMA; CHAIN: A, B; | PHOSPHOTRANSFERASE CAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT I CMK 3 (E.C.2.7.1.37) I CMK 4 | TRANSFERASE(PHOSPHOTR ANSFERASE) CAMP- DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (CAPK) LCTP 3 (CATALYTIC SUBUNIT) ICTP 4 | SERINEJTHREONINE. PROTEIN KINASE PAK- ALPHA; CHAIN: A, B; SERINEJTHREONINE. PROTEIN KINASE PAK- ALPHA; CHAIN: C, D; | FGF RECEPTOR 1; CHAIN: A, B; | FGF RECEPTOR 1; CHAIN: A, B; | PROTO-ONCOGENE TYROSINE-PROTEIN KINASE ABL: CHAIN: A. B: | HUMAN CYCLÍN- DEPENDENT KINASE 2; CHAIN: NULL; |
| SeqFold | | | | | | | | | |
| PMF score | | 60'0 | 0.37 | 0.48 | 0.89 | 0.22 | 0.33 | 0.51 | 0.7 |
| Verify score | | 0.32 | -0.11 | 0.18 | 0.35 | 0.14 | -0.07 | 0.12 | 0.26 |
| PSI- BLAST | | 1.50E-31 | 0 | 6.80E-97 | 6.80E-46 | 5.10E-31 | 7.00E-08 | 4.20E-06 | 1.70E-47 |
| End | | 396 | 434 | 434 | 397 | 344 | 372 | 372 | 399 |
| Start AA | | 163 | 122 | 122 | 148 | 147 | 506 | 761 | 146 |
| Chain ID | | ¥ | ш | ш | o o | В | £ | ¥ | |
| PDB ID | | lcm 8 | lcm k | lctp | 1f3m | lfgk | 1fgk | 1fbu | lhcl |
| SEQ ID NO: | | 596 | 296 | 296 | 989 | 965 | 596 | 986 | 296 |

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|------------------|--------------------------|---|--|---|--|--|--|--|---|--|---|
| PDB annotation | MITOSIS, PHOSPHORYLATION | SERINE/THREONINE-PROTEIN KINASE CSBP, RK, P38; PROTEIN SER/THR-KINASE, SERNE/THREONINE-PROTEIN KINASE | TRANSFERASE INK3; TRANSFERASE, INK3 MAP KINASE, SERINE/THREONINE PROTEIN 2 KINASE | TRANSFERASE INK3; TRANSFERASE, INK3 MAP KINASE, SERINETHREONINE PROTEIN 2 KINASE | KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION | KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION | TRÂNSFERASE MITOGEN ACTIVATED PROTEIN KINASE; TRANSFERASE, MAP KINASE, SERNDETRECONINE-PROTEIN KINASE, 2 P38 | KINASIP EABITI MUSCLE PHOSPHORYLASE KINASE; GLYCOGEN METABOLISM, TRANSEERASE, SERINETHEDNINE- PROTEIN, 2 KINASE, AFH-BINDING, CALMODULIA-BINDING | SERINE KINASE SERINE KINASE, TITIN, MUSCLE, AUTOINHIBITION | TRANSFERASE AAC; AMINOGINE 6'-N- ACETYLTRANSFERASE, ANTIBIOTIC 2 RESISTANCE, ACETYL COENZYME A | HYDROLASE ERA, GTPASE, RNA- BINDING, RAS-LIKE, HYDROLASE |
| Coumpound | | P38 MAP KINASE; CHAIN: NULL; | C-JUN N-TERMINAL KINASE; CHAIN: NULL; | C-JUN N-TERMINAL KINASE; CHAIN: NULL; | TWITCHIN; CHAIN: NULL; | TWITCHIN; CHAIN: A, B; | MAP KINASE P38, CHAIN: NULL; | PHOSPHORYLASE KINASE; CHAIN: NULL; | TITIN; CHAIN: A, B; | AMINOGLYCOSIDE N6- ACETYLTRANSFERASE TYPE 1; CHAIN: A; | GTP-BINDING PROTEIN ERA; CHAIN: A, B; |
| SeqFold score | | | | | | | | | | | |
| PMF | | 0.65 | 0.74 | 0.51 | 99.0 | 92.0 | 0.55 | 0.88 | 0.92 | 0.86 | 0.07 |
| Verify | | 0.1 | 0 | -0.12 | 0.15 | 0.31 | 0.09 | 0.22 | 0.16 | 0.38 | -0.81 |
| PSI- BLAST | | 1.40E-32 | 3.40E-34 | 7.00E-07 | 1.70E-53 | 6.80E-54 | 3.40E-36 | 1.70E-60 | 3.40E-41 | 0.0065 | 0.00039 |
| End | | 349 | 346 | 351 | 400 | 398 | 349 | 397 | 397 | 145 | 171 |
| Start | | 147 | 146 | 258 | 146 | 141 | 147 | 147 | 143 | 11 | 146 |
| Chain ID | | | | | | ¥ | | | V | V | V |
| PDB | | lian | 1jnk | ļi. | 1koa | Ikob | 1p38 | 1phk | 1tki | 1587 | lega |
| SEQ No: | | 965 | 965 | | 969 | 985 | 296 | 965 | 965 | 109 | 602 |

| | | | | | | _ | | | |
|------------------|---|---|---|--|---|---|---|---|-----------------------|
| PDB annotation | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGMIN ASSOCIATED 35 KDA PROTEIN, P35A, THREE HELIX BUNDLE | PHOSPHOTRANSFERASE RHOGAP DOMANI, HORSPHOTRANSFERASE, TPASE ACTIVATING PROTIEN, GAP, CDC42, 2 PHOSPHOINOSITIDE 3. KRNASE, SHB DOMANI, SHZ DOMANIN, SHOMAL, TRANSDICTION | PHOSPHOTRANSFERASE RHOGAP DOMANI, PHOSPHOTRANSFERASE, TPASE ACITY ATING PROTIEN, GAP, CDC42, 2 PHOSPHOINOSITIDE 3. KINASE, SHB DOMANI, SIR DOMANIN, SI SIGNAL, TRANSDICTION | PHOSPHOTRANSFERASE RHOGAP DOMANI, PHOSPHOTRANSFERASE, TPASE ACTIVATING PROTIEN, GAY, CDCA2, 2 PHOSPHOINOSTILDE 3. KINASE, SIB DOMANI, SIZ DOMANI, SIGNAL, TRANSHICTION | G-PROTEIN CDC42 GTPASE- ACTIVATING PROTEIN, G-PROTEIN, GAP, SIGNAL-TRANSDICTION | G-PROTEIN CDC42 GTPASE- ACTIVATING PROTEIN, G-PROTEIN, GAP, SIGNAL-TRANSDUCTION | COMPLEX(GTPASE ACTIVATURPROTO-COGENE) GTPASE-ACTIVATING PROTEIN RHOGAP, COMPLEX (GTPASE ACTIVATIONPROTO-ONCOGENE), GTPASE 2 TRANSITION STATE, GAP | COMPLEX(GTPASE ACTIVA/THVRPATO-OMOCGENE) GTPASE-ACTIVA/THING PROTEIN RHOGAP: COMPLEX (GTPASE ACTIVA/GTON/PROTO-OMCOGENE), GTPASE 7 TRANSTITIN STATE GAP | COMPLEX(GTPASE |
| Coumpound | SYNTAXIN-IA; CHAIN: A, B, C; | PHOSPHATIDYLINOSITOL 3- KINASE; CHAIN: A, B; | PHOSPHATIDYLINOSITOL 3- KINASE; CHAIN: A, B; | PHOSPHATIDYLNOSITOL 3- KINASE; CHAIN: A, B; | RHOGAP, CHAIN: NULL; | RHOGAP; CHAIN: NULL; | PSO-RHOGAP, CHAIN: A; TRANSFORMING PROTEIN RHOA; CHAIN: B; | P50-RHOGAP; CHAIN: A; TRANSFORMING PROTEIN RHOA; CHAIN: B; | P50-RHOGAP; CHAIN: A; |
| SeqFold score | | | | . – | 112.2 | | 118.67 | | |
| PMF | 0.07 | - | - | - | | - | | - | _ |
| Verify score | -0.14 | 0.43 | 0.78 | 0.77 | | 0.58 | | 0.54 | 0.9 |
| PSI- BLAST | 0.0039 | 1.30E-20 | . 1.30E-20 | 2.60E-40 | 1.80E-30 | 1.80E-30 | 9.10E-48 | 1.10E-30 | 9.10E-48 |
| End | 669 | 192 | 192 | 217 | 212 | 189 | 212 | 201 | 212 |
| Start | 260 | 25 | 25 | 25 | 13 | 16 | 51 | 16 | 91 |
| Chain ID | ¥ . | ∢ | В | щ | | | ¥ | ∢ | 4 |
| EDB ID | lez3 | 1pb w | 1pb w | Jpb w | lrgp | 1rgp | ltx4 | 104 | IX4 |
| SEQ D NO: | 909 | 909 | 605 | 605 | 909 | 909 | 902 | 509 | 905 |

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|-------------------------|---|---|--|--|--------------------------|----------------------------|------------------------|-----------------------------|------------|---|---|---|---|--|
| PDB annotation | ACTIVATN/PROTO-ONCOGENE) GTP-ASE-ACTIVATING PROTEIN RHOGAP; COMPLEX (GTPASE ACTIVATION/PROTO-ONCOGENE), GTPASE, 2 TRANSITION STATE, GAP | | MERCURY DETOXIFICATION MERCURY TRANSPORT PROTEIN; MERCURY DETOXIFICATION, PERPILASMIC, HEAVY METAL TRANSPORT, 2 ALPHA-BETA SANDWICH; | HYDROLASE COPPER- TRANSPORTING ATPASE, COPPER- BINDING DOMAIN, HYDROLASE | NIICLEAR IMPORT RECEPTOR | KARYOPHERIN ALPHA; NUCLEAR | LOCALIZATION SIGNAL, 2 | AUTOINHIBITION, INTRASTERIC | REGULATION | ARMADILLO REPEAT ARMADILLO REPEAT, BETA-CATENIN, CYTOSKELETON | | COMPLEX (TRANSFERASEPEPTIDE) COMPLEX (TRANSFERASEPEPTIDE) | COMPLEX (TRANSFERASEPEPTIDE) COMPLEX (TRANSFERASEPEPTIDE) | COMPLEX (TRANSFERASEPEPTIDE) ITAM PEPTIDE, COMPLEX (TRANSFERASEPEPTIDE), SYK, KINASE, SH2 DOMAIN, ITAM |
| Coumpound | TRANSFORMING PROTEIN RHOA; CHAIN: B; | | MERP; CHAIN: NULL; | MENKES COPPER- TRANSPORTING ATPASE; CHAIN: NULL; | IMPORTIN ALPHA: CHAIN: | Ą; | | | | BETA-CATENIN; CHAIN: NULL; | | C-SRC TYROSINE KINASE; CCHAIN: A, B; ACE-FORMYL PHOSPHOTYR-GLU-(N, N- DIPENTYL AMINE); CHAIN: C, D; | C-SRC TYROSINE KINASE; CHAIN: A, B; ACE-FORMYL PHOSPHOTYR-GLU-(N.N- DIPENTYL AMINE); CHAIN: C. D. | SYK KINASE, CHAIN: A, C, E, G, I, K; T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN; CHAIN: B, D, F, H, J, L; |
| SeqFold | | | | | | | | | | | | 172.37 | | |
| PMF score | | | , | _ | 0.46 | | | | | 96'0 | | | _ | - |
| Verify score | | | 0.86 | 0.81 | -0.02 | | | | | 0.42 | | | 1.07 | 0.57 |
| PSI- BLAST | | | 0.00026 | 0.0012 | 1.20E-06 | | | | | 0.00026 | | 6.50E-41 | 6.50E-41 | 7.80E-33 |
| End AA | | | 203 | 203 | 16 | | | | | 148 | | 255 | 255 | 255 |
| Start | | | 143 | 143 | 21 | | | | | 91 | | 150 | 150 | 126 |
| Chain | | | | | A | | | | | | | ¥. | 4 | V |
| SEQ PDB ID ID NO: | | | lafi | law0 | lial | | | | | 3bct | _ | 1a09 | 1a09 | 1381 |
| SEQ B B S | | | 909 | 909 | 909 | | | | | 909 | | 209 | 200 | 209 |

| PDB annotation | COMPLEX (TRANSFERASEPEPTIDE) ITAM PEPTIDE; COMPLEX (TRANSFERASEPEPTIDE), SYK, KINASE, SH2 DOMAIN, ITAM | | · | PROTEIN KINASE CDK2; PROTEIN KINASE, CELL CYCLE, PHOSPHORYLATION, STAUROSPORINE, 2 CELL DIVISION, MITOSIS, INHIBITION | COMPLEX (ISOMERASE/PROTEIN KINASE) FKBP12; SERINE/THREONINE-PROTEIN |
|-----------------|--|--|--|---|--|
| Coumpound | SYK KINASE; CHAIN: A, C, E, G, I, K; T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN; CHAIN: B, EPSILON CHAIN; CHAIN: B, | TRANSERBASE/PROSPHOTR ANSTERASIS OCAMPS DEPRODENT PROTEIN RINASE (ECAZ.1.37) (SCARKS) IAPM 3 ALPA ISOBEZYME ALPA ISOBEZYME ALPA ISOBEZYME THE PETRIOE LAWA (SI 38AS) COMPLEX WITH THE PETRIOE LAWA (SI 38AS) COMPLEX WITH THE DEPRODENT MEGA-8 INEM STATION PRICES AND INEM STATION PRICES AND INEM STATION PRICES AND INEM STATION PRICES AND INEM STATION PRICES INEM STATIO | TRANSPERASPHOSPHOTR ANSPERASP SCAAMPS- DEPENDENT PROTEIN SCARKS) LAPA (SCARKS) LAPA (SCARKS) LAPA ALPA ISOBUZYME (S1945) COMPLEX WITH THE PETITEDE LAMA S INTER DETERCENT MEGA-8 INTER DETERCENT MEGA-8 INTER DETERCENT MEGA-8 | CYCLIN-DEPENDENT PROTEIN KINASE 2; CHAIN: NULL; | FK506-BINDING PROTEIN; CHAIN: A. C. E. G; TGF-B SUPERFAMILY RECEPTOR |
| SeqFold | | 97.15 | | | 102.06 |
| PMF | 6.0 | | - | - | |
| Verify score | 0.26 | | | 0.34 | |
| PSI- BLAST | 1.30E-46 | 1.30E-35 | 1.305-35 | 1.30E-33 | 2.60E-74 |
| End | 372 | 542 | 515 | 529 | . 533 |
| Start | 151 | | 282 | 281 | 241 |
| Chain | 4 | ш | ш | | В |
| PDB DD | 1881 | Iap III | m m | laqi | 1960 |
| S e S | 209 | 607 | 607 | 607 | 607 |

| PDB annotation | KINASE RECEPTOR R4; COMPLEX (ISOMERASEPROTEIN KINASE), RECEPTOR 2 SERINE/THREONINE KINASE | COMPLEX (ISOMERASEPROTEIN KINASE) FRRPI; SERNDÉTRIEDANDE-PROTEIN KINASE RECEPTOR R4, COMPLEX (ISOMERASEPROTEIN KINASE), RECEPTOR 2 SERNDÉTHREONINE KINASE | V-SRC SH2 DOMAIN SRC SH2: V-SRC SH2 DOMAIN, PHOSPHOTYROSINE RECOGNITION DOMAIN, PP60 2 SRC SH2 DOMAIN | V-SRC SH2 DOMAIN SRC SH2, V-SRC SH2 DOMAIN, PHOSPHOTYROSINE RECOGNITION DOMAIN, PP60 2 SRC SH2 DOMAIN | COMPLEX (INHIBITOR PROTEING ASSISTANCE) PROTEIN, CYCLIA-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHANESET, COMPLEX (INHIBITOR PROTEIN/KINASE) | COMPLEX (INHIBITOR PROTEINGLASS) PROTEINGNEARS) NHIBITOR PROTEIN, CYCLIA-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHANEET, COMPLEX (INHIBITOR PROTEIN/KINASE) | | |
|-----------------|--|---|---|---|--|--|--|---|
| Coumpound | TYPE I; CHAIN: B, D, F, H; | FK506-BINDING PROTEIN, CHANI: A, G, G, TGF-B SUPERFAMILY RECEPTOR TYPE I, CHAIN: B, D, F, H; | PP60 V-SRC TYROSINE KINASE TRANSFORMING PROTEIN; CHAIN: NULL; | PP60 V-SRC TYROSINE KINASE TRANSFORMING PROTEIN; CHAIN: NULL; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B, | PHOSPHOTRANSFERASE CAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT ICMK 3 E.C. 27.1.371 ICMK | TRANSFERASE(PHOSPHOTR ANSFERASE) CAMP- DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (CAPK) ICTP 3 (CATALYTIC |
| SeqFold | | | | 165.48 | | 99.54 | | 99.49 |
| PMF | | - | _ | | | | | |
| Verify score | | 0.51 | 1.13 | | 99.0 | | 0.7 | |
| PSI- BLAST | | 2.60E-74 | 2.60E-40 | 2.60E-40 | 1.20E-34 | 1.20E-34 | 9.10E-35 | 6.50E-35 |
| End AA | | 531 | 259 | 263 | 529 | 538 | 515 | 542 |
| Start | | 256 | 155 | 155 | 269 | 270 | 282 | 227 |
| Chain ID | | В | | | ∢ | 4 | я | μ |
| PDB ID | | 1660 | PKI | 1bki | 1blx | 1blx | r i | letp |
| SEQ No: | | 607 | 209 | 209 | 209 | 209 | 607 | 209 |

| PDB annotation | | | TRANSFERASE KINASE DOMAIN, AUTOINHIBITORY FRAGMENT, HOMODIMER | PROTEIN KINASE CDK2; TRANSFERASE, SERINETHREONINE PROTEIN KINASE, ATP-BINDING, 2 CELL CYCLE, CELL DIVISION, MITOSIS, PHOSPHORYLATION | PROTEIN KINASE CDK2; TRANSFERASE, SERNETHEONINE PROTEIN KINASE, ATP-BINDING, 2 CELL CYCLE, CELL DIVISION, MITOSIS, PHOSPHORYLATION | TRANSFERASE INK3, TRANSFERASE, JNK3 MAP KINASE, SERINETHREONINE PROTEIN 2 KINASE | COMPLEX (TRANSFERASEPEPTIDE) SRC, SH3 DOMAIN, LIGANDS, NON- PEPTIDE ELEMENTS, 2 COMPLEX (TRANSFERASEPEPTIDE) | TRANSFERASE MITOGEN ACTIVATED PROTEIN KINASE, TRANSFERASE, MAP KINASE, SERINE/THREONINE-PROTEIN KINASE, 2 PR | |
|------------------|-----------------|--|---|--|--|---|--|--|---|
| Coumpound | SUBUNIT) 1CTP 4 | TRANSFERASE(PHOSPHOTR ANSFERASE) CAMP- DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (CAPK) ICTP 31 (CATALYTIC | SERNETHEONINE. PROTEIN KINASE PAK. ALPHA; CHAIN; A, B; SERNETHEONINE. PROTEIN KINASE PAK. | HUMAN CYCLIN- DEPENDENT KINASE 2; CHAIN: NULL; | HUMAN CYCLIN- DEFENDENT KINASE 2; CHAIN: NULL; | C-JUN N-TERMINAL KINASE; CHAIN: NULL; | C-SRC; CHAIN: C; NL1 (MN7- MN2-MN1-PLPPLP); CHAIN: N; | MAP KINASE P38; CHAIN: NULL; | PHOSPHOTRANSFERASE V. SRC TYROSINE KINASE TRANSFORMING PROTEIN (PHOSPHOTYROSINE ISHA 3 RECOGNITION DOMAIN |
| SeqFold score | | | | 111.67 | | | | | 165.79 |
| PMF | | _ | _ | | _ | _ | - | - | |
| Verify score | | 0.55 | 0.71 | | 0.43 | 9.0 | 0.13 | 0.44 | |
| PSI- BLAST | | 6.50E-35 | 1.30E-42 | 1.30E-37 | 1,30E-37 | 1.30E-33 | 2.60E-19 | 2,60E-32 | 9.10E-40 |
| End AA | | 515 | 519 | 538 | 529 | 538 | 149 | 212 | 256 |
| Start AA | | 282 | 272 | 273 | 281 | 569 | 88 | 269 | 154 |
| Chain | | ш | U | | | | ၁ | | ∢ |
| PDB ID | | Icp | 1Bm | Ibel | Ihol | ljnk | Inlo | 1p38 | 1sha |
| SEQ No: D | | 607 | 607 | 209 | 209 | 209 | 607 | 209 | 209 |

| PDB annotation | | | CYTOSKELETON CAPPING PROTEIN, CALCIUM-BINDING, DUPLICATION, REPEAT, 2 SH3 DOMAIN, CYTOSKELETON | CYTOSKELETON CAPPING PROTEIN, CALCIUM-BINDING, DUPLICATION, REPEAT, 2 SH3 DOMAIN, CYTOSKELETON | TRANSFERASE TRANSFERASE, TYROSINE KINASE, SH3, SH2, ONCOPROTEIN | TRANSFERASE TRANSFERASE, TYROSINE KINASE, SH3, SH2, ONCOPROTEIN | TYROSINE PHOSPHATASE SYP, SIFTP-2, TYROSINE PHOSPHATASE, INSULIN SIGNALING, SH2 PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA), ZINC |
|------------------|---|--|---|---|---|---|---|---|--|
| Coumpound | SH2) (E.C.2.7.1.112) COMPLEX WITH ISHA 4 PHOSPHOPETIDE A (TYR- VAL-PRO-MET-LEU, PHOSPHOR YLATED TYR) ISHA 5 | PHOSPHOTRANSERVASE SIC TROSINE KINASE TRANSFORMING PROTEIN (PHOSPHOTRXONE) ISHA 3 RECOGNITION DOMAIN SED) (E.C.Z.I.I.I.) SED) (E.C.Z.I.I.I.I.) SED) (E.C.Z.I.I.I.I.) SED) (E.C.Z.I.I.I.I.I.) SED) (E.C.Z.I.I.I.I.I.I.I.I.I.I.I.I.I.I.I.I.I.I | ALPHA-SPECTRIN; CHAIN: NULL; | ALPHA-SPECTRIN; CHAIN: NULL; | ABL TYROSINE KINASE; CHAIN: NULL; | ABL TÝROSINE KINASE; CHAIN: NULL; | SHP-2; CHAIN: A, B; | QGSR ZINC FINGER PEPTIDE, CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX |
| SeqFold score | | | | | 121.36 | | | | |
| PMF | | - | 0.89 | 0.01 | | 1 | 0.54 | 0.31 | 0.74 |
| Verify score | | | -0.02 | -0.25 | | 0.64 | -0.13 | -0.13 | 0 |
| PSI- BLAST | | 9.10E-40 | 1.30E-14 | 3.90E-09 | 9.10E-34 | 9.10E-34 | 6.50E-59 | 9.10E-21 | 1.30E-32 |
| End | | 256 | 991 | 130 | 255 | 255 | 425 | 284 | 290 |
| Start AA | | 154 | 100 | 75 | 62 | 80 | 75 | 203 | 209 |
| Chain ID | | ¥ | | | | | V | < | ٧ |
| PDB CI | | Isha | Ituc | 1tud | 2abi | 2abl | 2shp | lath | lalh |
| SEQ NO. | | 607 | 209 | 607 | 607 | 209 | 209 | 809 | 809 |

| PDB annotation | FINGER, DNA-BINDING PROTEIN | | | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX |
|------------------|---|--|--|--|--|--|--|---|
| Coumpound | OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | TRANSCRIFTION REGULATION YEAST TRANSCRIFTION PACTOR ADRI (RESIDUES 102 - 130) 1AKD 3 (AMINO TERMINAL ZINC FINGER DOMAIN) (NMR, 10 STRUCTURES) ARD 4 (ADRIB) 1AAD 5 | DNA-BINDING PROTEIN UNGAN BRHANGER. BINDING PROTEIN MBP-1 MUTANT WITH CYS 11 1BBO 3 REPLACED BY ABU (CILABU) (NMR, 60 STRUCTURES) 1BBO 4 | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F. G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; |
| SeqFold score | | | | | | | | |
| PMF | | 0.05 | 0.17 | 0.87 | - | _ | - | _ |
| Verify score | | -0.34 | -0.3 | 0.16 | 0.32 | 0.89 | 29.0 | 0.62 |
| PSI- BLAST | | 6.50E-05 | 2.60E-16 | 1.30E-22 | 6.50E-33 | 1.20E-42 | 5.20E-44 | 9.10E-47 |
| End | | 537 | 537 | 283 | 311 | 339 | 367 | 395 |
| Start AA | | 808 | 485 | 202 | | 259 | 286 | 314 |
| Chain ID | | | | ၁ | ပ | S | o . | ၁ |
| PDB CI | | lard | 1000 | Ime y | Jme y | Ime y | Jme y | m ~ |
| SEQ NO: | | 809 | 809 | 809 | 809 | 809 | 809 | 809 |

| PDB annotation | (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX | COMPLEX (ZINC FINGERDNA) ZINC COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CASYSTAL STRUCTINER, COMPLEX CATCLE COMPLEX CATCLES COMPLEX CATCLES COMPLEX CATCLES CAT | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA THERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA FINGER, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA THREACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) |
|-----------------|--|--|--|---|--|--|---|---|
| Coumpound | DNA; CHAÎN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAÎN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN; A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAÎN: A, B, D, E; CONSENSUS ZINO FINGER PROTEIN; CHAÎN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZING FINGER PROTEIN; CHAIN: C, F, G; |
| SeqFold | 102.94 | | | | | | | |
| PMF | | _ | | _ | | 0.22 | - | |
| Verify score | | 0.74 | 0.53 | 0.33 | 0.05 | -0.08 | 0.2 | 0.29 |
| PSI- BLAST | 9.10E-47 | 7.80E-46 | 1.30E-45 | 1.30E-40 | 2.60E-34 | 3.90E-32 | 3.90E-42 | 3.90E-46 |
| End | 396 | 423 | 451 | 479 | 202 | 589 | 617 | 645 |
| Start | 314 | 342 | 370 | | 426 | 454 | 536 | 564 |
| Chain TD | U | U | ပ | O | ပ | ပ | ပ | ပ |
| PDB CI | J. J | Jme y | Jme y | Jme y | J me | J. J | J me | Jme y |
| SE B SE | 809 | 809 | 809 | 809 | 809 | 809 | 809 | 809 |

| PDB annotation | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA THERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | ZINC FINGER TRANSCRIPTION FACTOR SP1; ZINC FINGER, TRANSCRIPTION ACTIVATION, SP1 | ZINC FINGER TRANSCRIPTION FACTOR SPI, ZINC FINGER, TRANSCRIPTION ACTIVATION, SPI | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASEB II, 2 TRANSCRIPTION NITIATION, ZNO FINGER PROTEIN | | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-YAIG I; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YYI, ZINC 2 FINGER REOTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION, INITIATIOR ELEMENT; YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN |
|------------------|---|--|--|--|--|---|--|---|
| Coumpound | DNA; CHAN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | SPIFS; CHAIN: NULL; | SPIP2; CHAIN: NULL; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TRANSCRIFTION REGULATION TRANSCRIPTIONAL ELONGATION FACTOR SII (FPIIS, NUCLEIC-ACID 17F13 BINDING DOMAIN) (NMR, 12 STRUCTURES) 1TF14 | YY'; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; |
| SeqFold score | | | | | 109.61 | | | |
| PMF | _ | _ | 0.01 | 0.13 | | 0.24 | 0.03 | 1 |
| Verify | 0.33 | 0.6 | -0.29 | -0.23 | | -0.22 | -0.34 | 0.26 |
| PSI- BLAST | 2.60E-46 | 2.60E-45 | 7.80E-05 | 9.10E-05 | 2.60E-71 | 0.0091 | 7.80E-29 | 6.50E-43 |
| End AA | 673 | 702 | 537 | 537 | 202 | 520 | 311 | 340 |
| Start | 592 | 620 | 509 | 509 | 342 | 480 | 165 | 229 |
| Chain | U | ပ | | | ⋖ | | ပ | ပ |
| 80 e | , me | , y | lsp1 | 1sp2 | 1416 | H | lubd 1 | Inbd |
| S e S | 809 | 809 | 809 | 809 | 809 | 809 | 809 | 809 |

| PDB annotation | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG I; TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC2 | FINGER PROTEIN, DNA-PROTEIN | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG I; | IKANSCRIPTION INITIATION, | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG I; | INITIATOR ELEMENT, YYI, ZINC2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (IRANSCRIPTION REGIT ATTOMONA) YING-YANG I: | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC2 |
|----------------|---|---|---|---|---|--------------------------------|------------------------|---------------------------|-------------------------------|-----------------------------|--------------------------------|------------------------|------------------------------|---------------------------|-----------------------------|------------------------|------------------------|------------------------------|-------------------------------|-----------------------------|------------------------|--------------------------------|--|---------------------------|-------------------------------|
| Coumpound | | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; | CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; | CHAIN: A, B; | | YY1; CHAIN: C; ADENO. | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS PS | CHAIN: A R. | 4 | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | CHAIN: A. B. | | | Orange of servine stark | ASSOCIATED VIRUS PS | INITIATOR ELEMENT DNA; | CHAIN: A, B; |
| SeqFold | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | | | | | | | | | | | - | | | | | 0.34 | | | | | 000 | 66.0 | | |
| Verify | | 0.55 | | 0.58 | | | 97.0 | | | | | 0.34 | | | | | -0.28 | | | | | 2 | 5 | | |
| PSI- BLAST | | 7.80E-52 | | 1.30E-53 | | | 5.20E-53 | | | | | 9.10E-51 | | | | | 2.60E-39 | | | | | 2000 | 2.2UE-45 | | |
| End | | 368 | | 395 | | | 451 | | | | | 479 | | | | | 589 | | | | | 210 | 010 | | |
| Start | | 263 | | 284 | | | 341 | | | | | 374 | | | | | 424 | | | | | 905 | 800 | | |
| Chain | | ၁ | | ပ | | | ၁ | | | | | ပ | | | | | 0 | | | | | C | ۔ | | |
| PDB | | lubd | | lubd | | | Inbd | | | | | 1ubd | | | | | 1ubd | | | | | 7 | 8 | | |
| SE O | | 809 | | 809 | | | 809 | | | | | 809 | | | | | 809 | | | | | 80,5 | 8 | | |

| | | т | - | , | | , | | , | _ |
|------------------|---|--|---|---|---|---|---|--|--|
| PDB annotation | FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATIONDALA) YING-YANG I; TRANSCRIPTION INITIATION, INITIATIOR ELEMENT. YYI, ZINO.2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION 3 COMPLEX TRANSCRIPTION AT THE TRANSCRIPTION AT THE TRANSCRIPTION AT T | COMPLEX (TRANSCRIPTION REGULATIONDNA) YNG-YANG I; TRANSCRIPTION INTLATION, INTLATOR ELEMENT YY, ZINO Z FINGER PROTEIN, DNA-PROTEIN RECOGNITION, SOMPLEX FINGEN PROTEIN, DNA-PROTEIN | TRANSCRIPTION REGULATION TRANSCRIPTION REGULATION, ADRI. ZINC FINGER, NMR | | | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINIDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING |
| Coumpound | | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO. ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | ADRI; CHAIN: NULL; | COMPLEX(TRANSCRIPTION REGULATION/DNA) TRAMTRACK PROTEIN (TWO ZINC-FINGER PEPTIDE) COMPLEXED WITH 2DRF 3 DNA 2DRF 4 | COMPLEX(TRANSCRIPTION REGULATION/DNA) TRAMTRACK RROTEIN (TWO ZINC-FINGER PEPTIDE) COMPLEXED WITH 2DRP 3 DNA 2DRP 4 | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; COMPLEX (DNA-BINDING |
| SeqFold score | | - | | | | | | | |
| PMF | | | - | 0.41 | 0.06 | 0.23 | - | - | - |
| Verify score | | -0.07 | 90.00 | -0.15 | 0.11 | 0.28 | 0.1 | 0.45 | 0.32 |
| PSI- BLAST | | 5.20E-56 | 1.30E-54 | 2.60E-18 | 1.30E-15 | 6.50E-18 | 9.10E-58 | 1.00E-65 | 1.30E-67 |
| End AA | | 674 | 101 | 509 | 530 | 563 | 369 | 397 | 480 |
| Start AA | | 564 | 990 | 455 | 479 | 505 | 230 | 259 | 314 |
| Chain | | ပ | O | | ∢ * | Ą | ¥ | ¥ | Ą |
| PDB DD | | lubd | lubd | 2adr | 2drp | 2drp | 2gli | 2gli | 2gli |
| Š e Š | | 809 | 809 | 809 | 809 | 809 | 809 | 809 | 88 |

| PDB annotation | PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (GTPASE- ACTIVATINGGTP-BINDING) COMPLEX (GTPASE- ACTIVATINGGTP-BINDING), GTPASE ACTIVATION | TRANSPORT PROTEIN TC4; GTPASE, NUCLEAR TRANSPORT, TRANSPORT PROTEIN | TRANSPORT PROTEIN TC4; GTPASE, NUCLEAR TRANSPORT, TRANSPORT PROTEIN | SIGNALING PROTEIN PROTEIN- PROTEIN COMPLEX, ANTIPARALLEL COILED-COIL | SIGNALING PROTEIN PROTEIN- PROTEIN COMPLEX, ANTIPARALLEL COILED-COIL | SIGNALING PROTEIN P21-RAC2; RHO GDI 2, RHO-GDI BETA, LY-GDI; BETA |
|-----------------|--|--|--|--|--|--|---|---|--|--|--|
| Coumpound | CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLJI; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA: CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | PSO-RHOGAP, CHAIN: A, B, C, CDC42HS; CHAIN: D, E, F; | GTP-BINDING PROTEIN RAN; CHAIN: A, B; | GTP-BINDING PROTEIN RAN; CHAIN: A, B; | HIS-TAGGED TRANSFORMING PROTEIN RHOA(0-181); CHAIN: A; PKN; CHAIN: B; | HIS-TAGGED TRANSFORMING PROTEIN RHOA(0-181); CHAIN: A; PKN: CHAIN: B: | RAS-RELATED C3 BOTULINUM TOXIN |
| SeqFold | | | | | 92.71 | | 55.55 | - | 61.64 | | |
| PMF | | 0.37 | - | 0.99 | | _ | | 99:0 | | - . | |
| Verify score | | 0 | 0.3 | 0.16 | | 0.46 | | 0.15 | | 0.19 | 0.14 |
| PSI- BLAST | | 1.30E-56 | 1.30E-64 | 2.60E-70 | 2.60E-70 | 2.60E-20 | 3.90E-24 | 3.90E-24 | 1.30E-20 | 1.30E-20 | 2.60E-20 |
| End AA | | 619 | | 101 | 703 | 165 | 192 | 181 | 187 | 170 | 172 |
| Start AA | | 398 | 536 | 564 | 564 | 9 | - | 9 | | 9. | 9 |
| Chain ID | | V | < | V | ٧ | D | В | В | V | V | ν. |
| PDB ID | | 2gli | 2gli | 2gli | 2gli | lam 4 | lbyu | Ibyu | lexz | lexz | 1ds6 |
| SEQ NO: | | 809 | 809 | 809 | 809 | 609 | 609 | 609 | 609 | 609 | 609 |

| | | | | | | | | | | | _ | |
|------------------|---|--|--|--|---|---|--|--|---|---|--|---|
| PDB annotation | SANDWHICH, PROTEIN-PROTEIN COMPLEX, G-DOMAIN, 2 IMMUNOGLOBULIN FOLD, WALKER FOLD, GTP-BINDING PROTEIN | G PROTEIN G PROTEIN, RAS, ARF, ARF6, MEMBRANE TRAFFIC | PROTEIN TRANSPORT GDP-BINDING, MEMBRANE TRAFFICKIN, NON- MYRISTOYLATED 1HUR 16 | PROTEIN TRANSPORT GDP-BINDING, MEMBRANE TRAFFICKIN, NON- MYRISTOYLATED IHUR 16 | SMALL GTPASE KARYOPHERIN BETA, P95 SMALL GTPASE, NUCLEAR TRANSPORT RECEPTOR | SMALL GTPASE KARYOPHERIN BETA, P95 SMALL GTPASE, NUCLEAR TRANSPORT RECEPTOR | GTP-BINDING GTP-BINDING, GTPASE, SMALL G-PROTEIN, RHO FAMILY, RAS SUPER 2 FAMILY | GTP-BINDING GTP-BINDING, GTPASE, SMALL G-PROTEIN, RHO FAMILY, RAS SUPER 2 FAMILY | COMPLEX (SMALL GIPASENUCLEAR PROTEIN) COMPLEX (SMALL GIPASENUCLEAR PROTEIN), SMALL GIPASE, 2 NUCLEAR TRANSPORT | COMPLEX (SMALL GTPASENUCLEAR PROTEIN) COMPLEX (SMALL GTPASENUCLEAR PROTEIN), SMALL GTPASE, 2 NUCLEAR TRANSPORT | COMPLEX(GTPASE ACTIVA TUNPROTO-ONCOGENE) GTPASE-ACTIVA TING PROTEIN RHOGAP, COMPLEX (GTPASE ACTIVA GTIONRO TOTO-ONCOGENE), GTPASE, 2 TRANSITION STATE, GAP | COMPLEX(GTPASE ACTIVATN/PROTO-ONCOGENE) GTPASE-ACTIVATING PROTEIN |
| Coumpound | SUBSTRATE 2; CHAIN: A; RHO GDP-DISSOCIATION INHIBITOR 2; CHAIN: B; | ADP-RIBOSYLATION FACTOR 6, CHAIN: A; | HUMAN ADP- RIBOSYLATION FACTOR 1; IHUR 5 CHAIN: A, B; IHUR 7 | HUMAN ADP- RIBOSYLATION FACTOR 1; IHUR 5 CHAIN: A, B; IHUR 7 | RAN; CHAIN: A, C; IMPORTIN BETA SUBUNIT; CHAIN: B, D; | RAN; CHAIN: A, C; IMPORTIN BETA SUBUNIT; CHAIN: B, D; | RAC1, CHAIN: NULL; | RACI; CHAIN: NULL; | RAN; CHAIN; A, C; NUCLEAR PORE COMPLEX PROTEIN NUP358; CHAIN: B, D; | RAN; CHAIN; A, C; NUCLEAR PORE COMPLEX PROTEIN NUP358; CHAIN: B, D; | P50-RHOGAP, CHAIN: A; TRANSFORMING PROTEIN RHOA; CHAIN: B; | P50-RHOGAP, CHAIN: A; TRANSFORMING PROTEIN RHOA; CHAIN: B; |
| SeqFold score | | | 55.9 | | 71.05 | | 52.65 | | 77.78 | | 54.35 | |
| PMF | | 0.57 | | 0.55 | | 66.0 | | - | | 9.0 | | _ |
| Verify score | | 0.12 | | -0.12 | | 9.04 | | 0.36 | | -0.02 | | 0.37 |
| PSI- BLAST | | 1.20E-22 | 7.80E-23 | 7.80E-23 | 3.90E-23 | 3.90E-23 | 3.90E-21 | 3.90E-21 | 9.10E-24 | 9.10E-24 | 2.60E-20 | 2.60E-20 |
| End | | 168 | 172 | 891 | 174 | 173 | 189 | 171 | 187 | 180 | 185 | 165 |
| Start | | 9 | _ | vo | 3 | 9 | 2 | ٥ | m | 9 | 6 | S. |
| Chain ID | | 4 | V | A | A | 4 | | | ၁ | ၁ | В | В |
| PDB CD | | 1e0s | Ihur | Ihur | libr | riji. | 直 | 1mh I | Іпр | Ę | 1114 | lb4 |
| SEQ B B SE | | 609 | 609 | 609 | 609 | 609 | 609 | 609 | 609 | 609 | 609 | 609 |

| PDB annotation | RHOGAP, COMPLEX (GTPASE ACTIVATION/PROTO-ONCOGENE), GTPASE, 2 TRANSITION STATE, GAP | COMMUNICATION AND THE PROPERTY. | COMPLEX (INHIBITOR PROTEIN/KINASE) INHIBITOR | PROTEIN, CYCLIN-DEPENDENT | KINASE, CELL CYCLE 2 CONTROL, | ALPHA/BELA, COMPLEX (INHIBITOR PROTEIN/KINASE) | PROTEIN KINASE CDK2; | TRANSFERASE, SERINE/THREONINE | CELL CYCLE, CELL DIVISION | MITOSIS, PHOSPHORYLATION | UBIQUITIN CONJUGATION UBC2; | UBIQUITIN CONJUGATION, | TICAGE TIPLOTHERY TIPLOTHERY | CONTIGATING ENZYME YEART | (IRIOI IITIN CONTIGATION LIBCI- | UBIQUITIN CONJUGATION, LIGASE | MUSCLE PROTEIN CTNC; CARDIAC, MUSCLE PROTEIN, REGULATORY. | CALCIUM BINDING | HYDROLASE CALCINEURIN; | HIDROLASE, FROSFHAIASE, IMMUNOSUPPRESSION | CALCIUM-BINDING PROTEIN | CALCIUM-MYRISTOYL SWITCH, | CALCUIM-BINDING PROTEIN | CALCIUM-REGULATED MUSCLE | CONTRACTION CALCITIM-BINIDING | TROPONIN E-F HAND 2 OPEN | CONFORMATION REGULATORY | DOMAIN, CALCIUM-REGULATED 3 | MUSCLE CONTRACTION | CALCTUM-BINDING PROTEIN EF- |
|------------------|---|---------------------------------|---|---------------------------|-------------------------------|---|----------------------|-------------------------------|---------------------------|--------------------------|-----------------------------|---------------------------|------------------------------|--|---------------------------------|-------------------------------|--|-----------------|------------------------|--|-------------------------|---------------------------|-------------------------|--------------------------|-------------------------------|--------------------------|-------------------------|-----------------------------|--------------------|-----------------------------|
| Coumpound | | | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; | P19INK4D; CHAIN: B; | | | HUMAN CYCLIN- | DEPENDENT KINASE 2; | CHAIN: NULL; | | UBIQUITIN-CONJUGATING | ENZYME KAD6; CHAIN: A, B, | L; | UBIQUITIN CONJUGATING FNZYMP: CHAIN: A: | I IBTO IIITIN CONTI GATING | ENZYME; CHAIN: NULL; | TROPONIN C; CHAIN: NULL; | | SERINE/THREONINE | A, B; | RECOVERIN; CHAIN: NULL; | | | TROPONIN C; CHAIN: NULL; | | | | | | TROPONIN C; 17NX 4 |
| SeqFold score | | | 129.83 | | | | 118.75 | | | | 54.69 | | 2107 | 24.8/ | 50 33 | 20.00 | 70.38 | | 78.45 | | 67.12 | | | 68.38 | | | | | | 67.26 |
| PMF | | | | | | | | | | | | | | | Ī | | | | | | | | | | | | | | | |
| Verify score | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PSI- BLAST | | 100 | 2.60E-52 | | | | 7.80E-50 | | | | 1.00E-15 | | 107.0 | 7.90E-17 | 2 60E-14 | | 5.20E-06 | | 7.80E-21 | | 5.20E-20 | | | 9.10E-17 | | | | | | 1.20E-16 |
| End AA | | 1 | 169 | | | | 687 | | | | 337 | | 3,16 | č | 333 | | 468 | | 476 | | 491 | | - | 465 | | | | | | 463 |
| Start | | | 370 | | | | 371 | | | | 167 | | | 801 | 167 | | 317 | | 320 | | 311 | | | 320 | | | | | | 320 |
| Chain | | | ∢ | _ | | | | | | | ٧ | _ | | ₹ | | | | | В | | | | | | | | | | | |
| PD8 | | | Iblx — | | | | 골 | | | | layz | | 1 | <u>8</u> | Jask | | laj4 | | laui | | liku | | | Itef | | | | | | Iţx |
| S e S | | 1 | 612 | | | | 612 | | | | 628 | | 95 | 979 | 869 | 0.00 | 169 | | 189 | | 631 | | | E8 | | | | | | 8 |

| PDB annotation | HAND ITNX 14 | PHOSPHOTRANSFERASE PHOSPHOTRANSFERASE | | PHOSPHOTRANSFERASE NUCLEOSIDE TRIPHOSPHATE, NUCLEOSIDE DIPHOSPHATE INUE 10 | COMPLEX (GTPASE- ACTIVATINGGIP-BINDING) COMPLEX (GTPASE- ACTIVATING/GIP-BINDING), GTPASE ACTIVATION | SIGNALING PROTEIN GTP-BINDING PROTEINS, PROTEIN-PROTEIN COMPLEX, EFFECTORS | SIGNALING PROTEIN GTP-BINDING PROTEIN RHOA, GTPASE RHOA; RHO GDI 1; RHO GTPASE, G-PROTEIN, SIGNALING PROTEIN | SIGNALING PROTEIN G PROTEIN, GTP HYDROLYSIS, KINETIC CRYSTALLOGRAPHY, 2 SIGNALING PROTEIN | SIGNALING PROTEIN PROTEIN- PROTEIN COMPLEX, ANTIPARALLEL COILED-COIL | SIGNALING PROTEIN P21-RAC2; RHO GDI 2, RHO-GDI BETA, LY-GDI; BETA SANDWHICH, PROTEIN-PROTEIN COMPLEX, G-DOMAIN, POI JAI KFP NAMINOGI ORITI N FOI D. WAI KFP | FOLD, GTP-BINDING PROTEIN |
|-----------------|---------------------|---|---|--|---|---|---|--|--|---|---------------------------|
| Coumpound | CHAIN: NULL; ITNX 5 | NUCLEOSIDE DIPHOSPHATE TRANSFERASE; CHAIN: A, B, C; | PHOSPHOTRANSFERASE NUCLEOSIDE DIPHOSPHATE KINASE (E.C.2.7.4.6) INSQ 3 | NUCLEOSIDE DIPHOSPHATE KINASE; INUE 4 CHAIN: A, B, C, D, E, F; INUE 5 | P50-RHOGAP, CHAIN: A, B, C; CDC42HS, CHAIN: D, E, F; | RAS-RELATED PROTEIN RAP-1A; CHAIN: A; PROTO- ONKOGENE SERINE/THREONINE PROTEIN KINASE CHAIN: B: | TRANSFORMING PROTEIN RHOA; CHAIN: A, C, RHO GDP DISSOCIATION INHIBITOR ALPHA; CHAIN: E, F. | TRANSFORMING PROTEIN P21/H-RAS-1; CHAIN: A; | HIS-TAGGED TRANSFORMING PROTEIN RHOA(0-181); CHAIN: A; PKN: CHAIN: B: | RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE 2; CHAIN: A; RHO GDP-DISSOCIATION NHIRITOR 2; CHAIN: R. | minute on 2, orman, D, |
| SeqFold | | 105.78 | 104.27 | 105.45 | | | | | | | |
| PMF | | | | | 0.55 | 0 | 0.65 | 0.36 | 0.93 | 0.54 | |
| Verify score | | | | | 0.31 | 0.17 | 0.24 | 0.23 | 0.39 | 0.05 | |
| PSI- BLAST | | 3.60E-53 | 3.60E-50 | 9.00E-53 | 3.60E-56 | 5.40E-56 | 9.00E-62 | 1.80E-59 | 9.00E-62 | 1.40E-62 | |
| End | П | 113 | 115 | 116 | 263 | 264 | 271 | 265 | 264 | 267 | |
| Start AA. | | - | _ | - | 88 | 98 | 68 | 98 | 68 | 88 | |
| Chain ID | | V | A | ٧ | Ω | ¥ | Ą | Y | ¥ | 4 | |
| PDB ID | П | lbc4 | Insq | Inuc | lam 4 | 1c1y | Icc0 | lotq | lcxz | Jds6 | |
| S a S | | 949 | 949 | 646 | 658 | 859 | 858 | 859 | 859 | 858 | |

| DB Chain Shr1 Pad FSI- Varigh PMF SeqPelad Coumpound FPD B annotation 658 1b D AA ABLAST secre 54:39 HUMAN ADP- REACTOR I. FROTENTRANSPORT GDP-BINDING. 658 1bm A 526 130E-56 0.19 0.45 RACI, GHAIN NULL; SNALL G-PROTEN RADIOSON GORDER 658 1bm 88 267 130E-56 0.19 0.45 RACI, GHAIN NULL; SNALL G-PROTEIN REPEACH, VION- RAGIOL GORDER 658 1bm 88 267 130E-56 0.11 0.45 RACI, GHAIN NULL; SNALL G-PROTEIN 658 1bg A 88 207 120E-66 0.01 0.4 GOAGAGAGAGAGAGAGAGAGAGAGAGAGAGAGAGAGAGA | | | | | | | | | | | |
|---|----------------|--|--|--|--|--|--|---|---|---|--------------------------|
| PDB Chain Shart End FS1. Verify PMF Soqvoid | PDB annotation | PROTEIN TRANSPORT GDP-BINDING, MEMBRANE TRAFFICKIN, NON- MYRISTOYLATED 1HUR 16 | GTP-BINDING GTP-BINDING, GTPASE, SMALL G-PROTEIN, RHO FAMILY, RAS SUPER 2 FAMILY | COMPLEX(GTPASE ACTIVATURPROTO-ONCOGENE) GTPASE-ACTIVATING PROTEIN RHOGAP, COMPLEX (GTPASE ACTIVATIONPROTO-ONCOGENE), GTPASE, 2 TRANSITION STATE, GAP | HYDROLASE CDC42/CDC42GaP: CDC42/CDC42GAP; TRANSITION STATE, G-PROTEIN, GAP, CDC42, ALF3., HYDROLASE | HYDROLASE G PROTEIN, VESICULAR TRAFFICKING, GTP HYDROLYSIS, RAB 2 PROTEIN, NEUROTRANSMITTER RELEASE, HYDROLASE | TRANSCRIPTION REGULATION PROTO-ONCOGENE, NUCLEAR BODIES (PODS), LEUKEMIA, 2 TRANSCRIPTION REGILI ATION | | LIGASE CBL, UBCH7, ZAP-70, E2, UBQUITIN, E3, PHOSPHORYLATION, 2 TYROSINE KINASE, UBQUITINATION, PROTEIN DEGRADATION, | METAL BINDING PROTEIN RING FINGER PROTEIN MATI; RING FINGER (C3HC4) | HELICASE DNA REPAIR, DNA |
| PDB Chain Shart Ead PSI; Verify PMF | Coumpound | HUMAN ADP- RIBOSYLATION FACTOR 1; IHUR 5 CHAIN: A, B; IHUR 7 | RACI; CHAIN: NULL; | P50-RHOGAP, CHAIN: A; TRANSFORMING PROTEIN RHOA; CHAIN: B; | GTP BINDING PROTEIN (G25K); CHAIN: A; GTPASE ACTIVATING PROTEIN (RHG); CHAIN: B; | Rab3a; Chain: A; | TRANSCRIPTION FACTOR PML; CHAIN: NULL; | VIRUS EQUINE HERPES VIRUS-I (C3HC4, OR RING DOMAIN) ICHC 3 (NMR, 1 STRUCTURE) ICHC 4 | SIGNAL TRANSDUCTION PROTEIN CBL; CHAIN: A; ZAP-70 PETTIDE, CHAIN: B; UBIQUITIN-CONJUGATING ENZYME E12-18 KDA UBCH7; CHAIN: C; | CDK-ACTIVATING KINASE ASSEMBLY FACTOR MAT1; CHAIN: A; | PCRA; CHAIN: NULL; |
| PDB Chalin Shart End PSI; Verify | SeqFold | 54.59 | | | | | | | | | |
| PDB Chain Shart End PSI- Verify | PMF | | 0.45 | 0.82 | 0.4 | 0.47 | 0.25 | 86:0 | 6.0 | 60.0 | 0,21 |
| PDB Chain Shart End | Verify | | 0.19 | . 0.31 | -0.01 | 0.11 | -0.73 | 0.24 | 0.25 | -0.44 | |
| 103 Chain Shart 1 1 1 1 1 1 1 1 1 | PSI- BLAST | 7.20E-11 | 1.30E-63 | 1.80E-58 | 7.20E-60 | 1.10E-54 | 9.00E-06 | 9.00E-15 | 1.80E-10 | 1.30E-05 | 0.002 |
| 100 100 | End AA | 266 | 267 | 263 | 270 | 265 | 59 | 9 | 99 | 72 | 218 |
| PDB DD I hur I hur I hur I hur I led- I led- I lebor | Start | 75 | 88 | 68 | 88 | 98 | 91 | 16 | 81 | 18 | 172 |
| | Chain D | 4 | | а | V | < | | | ¥ | V | |
| | PDB DD | Thur. | 重 | 1tx4 | 2ngr | 3rab | 1bor | 1chc | 1fbv | 1g25 | ē |
| | Se Si | 658 | 658 | 658 | | 658 | 659 | 629 | 629 | 629 | |

| | | | | , | _ | | | | | , |
|----------------|--|--|--|--|---|---|---|---|---|-----------------------------|
| PDB annotation | REPLICATION, SOS RESPONSE, HELLCASE, 2 ATP-BINDING, DNA- BINDING | HELICASE DNA REPAIR, DNA REPLICATION, SOS RESPONSE, HELICASE, ATP-2 BINDING, DNA- BINDING | COMPLEX (HELICASE/DNA) COMPLEX (HELICASE/DNA), HELICASE, DNA UNWINDING | HYDROLASEDNA ATP-DEPENDENT HELICASE PERA, HELICASE PERA, HELICASE PERA, HYDROLASE, DNA, PRODUCT COMPLEX | | TRANSCRIPTION HELIX-BUNDLE | TRANSCRIPTION HELIX-BUNDLE | | | |
| Соитроипа | | PCRA (SUBUNIT); CHAIN: A; PCRA (SUBUNIT); CHAIN: B; PCRA (SUBUNIT); CHAIN: C; PCRA (SUBUNIT); CHAIN: D; | ATP-DEPENDENT DNA HELICASE REP; CHAIN: A, B; DNA CHAIN: C; | HELICASE PCRA, CHAIN: A, P. HELICASE PCRA; CHAIN: B, G, DNA (3. DPTP-PTP-PT-7.3); CHAIN: CHAIN: CHAIN: CHAIN: CHAIN: H, DNA (3. CPR-PTP-PTP-7.3); CHAIN: H, DNA (4. CPR-C)-3); CHAIN: H, C | | TRANSCRIPTION ELONGATION FACTOR S-II; CHAIN: A: | TRANSCRIPTION ELONGATION FACTOR S-II; CHAIN: A; | TRANSCRIFTION TRANSCRIPTIONAL ELONGATION FACTOR SII (FITIS, NUCLEIC-ACID ITF13 BINDING DOMANI) (NMR, 12 STRUCTIRES) ITF14 | TRANSCRIPTION TRANSCRIPTION TRANSCRIPTIONAL ELONGATION FACTOR SII (FIFIS, NUCLEIC-ACID ITFI 3 BINDING DOMAIN) (NMR, 12 STRUCTURES) ITFI 4 | TRANSCRIPTION REGULATION |
| SeqFold | | | | | | | | | 84.88 | |
| PMF | | 0.28 | 0.69 | 0.88 | | 0.24 | 0.18 | - | | 1 |
| Verify | | -0.84 | -0.67 | -0.31 | | -0.43 | 0.45 | 0.45 | | 0.45 |
| PSI- BLAST | | 0.0045 | 0.00011 | 9.00E-06 | | 1.00E-18 | 3.60E-12 | 1.30E-22 | 3.90E-24 | 3.90E-24 |
| End AA | | 202 | 238 | 236 | | 49 | 49 | 332 | 332 | 332 |
| Start | | 172 | 172 | 172 | | - | 4 | 283 | 283 | 283 |
| Chain | | B | 4 | ∢ | | ∢ | V | | | |
| PDB DD | | 1qhg | luaa | 2pjr | | leo0 | leo0 | 9 | 91 | Ē |
| S a S | | 199 | 199 | 199 | | £99 | E99 | E99 | 699 | 663 |

| | | _ | | | | | | _ | | | | | _ | | _ | | | _ | | | | | | | | | |
|------------------|--|---|--|--|-------------------------------|--------------------------------|--------------------------------------|-------------------------|------------------------------|-------------------------------|----------------------------------|------------------------------------|-------------------------|------------------------------|-------------------------------|-----------------------|-------------|-------------------------|------------------------------|-------------------------------|--------------------------------|-----------------------------|-------------|------------------------------|------------------------|---------------------|------------------------|
| PDB annotation | | | RNA BINDING PROTEIN/RNA XLRBAP, ROTGEN/RNA COMPLEX, DOUBLE STRANDED RNA, PROTEIN- RNA 2 INTERACTIONS, RNA-BINING PROTEIN/RNA BINDING | RNA BINDING PROTEIN/RNA XI.RBPA: PROTEIN-RNA COMPI.EX | DOUBLE STRANDED RNA, PROTEIN- | RNA 2 INTERACTIONS, RNA-BINING | PROTEIN, RNA BINDING PROTEIN/RNA | RNA BINDING PROTEIN/RNA | XLRBPA; PROTEIN-RNA COMPLEX, | DOUBLE STRANDED RNA, PROTEIN- | KNA Z INI EKACI IONS, KNA-BINING | PROTEIN, KNA BINDING PROTEINRNA | RNA BINDING PROTEIN/RNA | XLRBPA; PROTEIN-RNA COMPLEX, | DOUBLE STRANDED RNA, FROIEIN- | DEOTEN DNA DRIDING | PROTEIN/RNA | RNA BINDING PROTEIN/RNA | XLRBPA; PROTEIN-RNA COMPLEX, | DOUBLE STRANDED RNA, PROTEIN- | RNA 2 INTERACTIONS, RNA-BINING | PROTEIN, RNA BINDING | PROTEIN/RNA | CELL CYCLE/RNA DSRBDIII; NMR | DARRO DROSOPHILA RNA 2 | HAIRPIN | |
| Coumpound | TRANSCRIPTIONAL ELONGATION FACTOR SII (FIES, NUCLEIC-ACID 1TFI 3 BINDING DOMAIN) (NMR, 12 STRUCTURES) 1TFI 4 | | DOUBLE STRANDED RNA BINDING PROTEIN A; CHAIN: A, B, RNA (5* R(*GP*GP*CP*CP*GP*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP | DOUBLE STRANDED RNA BINDING PROTEIN A: | CHAIN: A, B; RNA (5'- | R(*GP*GP*CP*GP*CP*GP*CP | *GP*CP*C)-3'); CHAIN: C, D, E, G: | DOUBLE STRANDED RNA | BINDING PROTEIN A; | CHAIN: A, B; RNA (5'- | K(*GF*GF*CF*GF*CF*GF*CF | E, G; | DOUBLE STRANDED RNA | BINDING PROTEIN A; | D/*CD*CD*CD*CD*CD*CD*CD | *GP*CP*C)-3%-CHAIN: C | E.G. | DOUBLE STRANDED RNA | BINDING PROTEIN A; | CHAIN: A, B; RNA (5'- | R(*GP*GP*CP*GP*CP*GP*CP | *GP*CP*C)-3'); CHAIN: C, D, | E, G, | MATERNAL EFFECT | CHAIN: A: STAILEEN | DOUBLE-STRANDED RNA | BINDING DOMAIN; CHAIN: |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF score | | | 0.99 | 0.42 | | | | 66.0 | | | | | 0.39 | | | | | 0.7 | | | | | | 0.31 | | | |
| Verify score | | | 90:0 | 0.45 | | | | 0.11 | | | | | -0.16 | | | | | 90.0 | | | | | | -0.12 | | | |
| PSI- BLAST | | | 1.60E-13 | 1.30E-14 | | | | 2.60E-16 | | | | | 1.80E-09 | | | | | 1.60E-07 | | | | | | 1.80E-14 | | | |
| End | | | 452 | 451 | | | | 574 | | | | | 829 | | | | | 452 | | | | | į | 454 | | | |
| Start AA | | | 388 | 390 | | | | 512 | | | | | 514 | | | | | 888 | | | | | | 380 | | | |
| Chain | | | ∢ | ٧ | | | | ¥ | | | | | Ą | | | | | В | | | | | | < | | | |
| EDB CD | | | Idi2 | ZIPI | | | | 1di2 | | | | | 1472 | | | | | ZIPI | | | | |] | lekz | | | |
| SEQ No. de | | | 999 | 999 | _ | | | 664 | | | | | 664 | | | | | 664 | | | | | | 99 | | | |

| PDB annotation | | CELL CYCLERNA DSRBDIII, NMR STRUCTURE, PROTEINTRAA, PROTEIN DSRBD, DROSOPHILA, RNA 2 HAIRPIN | CELL CYCLERNA DSRBDIII, NMR STRUCTURE, PROTEINRAA, PROTEIN DSRBD, DROSOPHILA, RNA 2 HAIRPIN | CELL CYCLERNA DSRBDII; NMR STRUCTURE, PROTEINRAA, PROTEIN DSRBD, PROSOPHILA, RNA 2 HAIRPIN | TRANSFERASE DSRNA-BINDING DOMAIN, NMR, PKR, SOLUTION STRUCTURE, PROTEIN 2 KINASE, TRANSFERASE | TRANSFERASE DSRNA-BINDING DOMAIN, NMR, PKR, SOLUTION STRUCTURE, PROTEIN 2 KINASE, TRANSFERASE | DOUBLE STRANDED RNA BINDING DOMAIN STAUFEN ISTU 13 | DOUBLE STRANDED RNA BINDING DOMAIN STAUFEN 1STU 13 | DOUBLE STRANDED RNA BINDING DOMAIN STAUFEN ISTU 13 | RNA-BINDING PROTEIN/RNA TRA PRE-MRNA, SPLICING REGULATION, RNP DOMAIN, RNA COMPLEX | GENE REGULATION/RNA POLY(A) BINDING PROTEIN 1, PABP 1; RRM, |
|------------------|----|---|--|---|--|--|---|---|---|--|--|
| Coumpound | B. | MATERNAL EFFECT PROTEIN (STAUFEN); CHAM: A; STAUFEN DOUBLE-STRANDED RNA BINDING DOMAIN; CHAIN: B: | MATERNAL EFFECT PROTEIN (STAUFEN); CHAN: A; STAUFEN DOUBLE-STRANDED RNA BINDING DOMAIN; CHAIN: | MATERNAL BFFECT PROTEIN (STAUFEN); CHAM: A; STAUFEN DOUBLE-STRANDED RNA BINDING DOMAIN; CHAIN: B: | PROTEIN KINASE PKR; CHAIN: A; | PROTEIN KINASE PKR; CHAIN: A: | MATERNAL EFFECT PROTEIN STAUFEN; 1STU 4 | MATERNAL EFFECT PROTEIN STAUFEN: 1STU 4 | MATERNAL EFFECT PROTEIN STAUFEN; 1STU 4 | SXL-LETHAL PROTEIN; CHAIN: A, B; RNA (5'- RP*GP*UP*GP*UP*UP*U P*UP*UP*UP*UP*UP-UP- P* O: | POLYDENYLATE BINDING PROTEIN I; CHAIN: A, B, C, |
| SeqFold score | | | | | | | | | | | |
| PMF score | | 0.69 | 0.39 | - | 0.06 | 60:0 | 0.07 | _ | 0.11 | 0.92 | _ |
| Verify score | | 90:0- | 0.04 | 0.75 | -0.17 | -0.05 | 0.23 | 0.19 | -0.24 | 0.48 | 1.05 |
| PSI- BLAST | | 5.20E-15 | 5.40E-05 | 1.30E-19 | 1.10E-15 | 7.20E-08 | 3.60E-13 | 3.90E-18 | 0.0009 | 1.305-10 | 9.10E-11 |
| End | | 451 | 557 | 574 | 469 | 558 | 454 | 575 | 557 | 84 | 88 |
| Start AA | | 384 | 209 | 511 | 375 | 518 | 388 | 512 | 514 | _ | 01 |
| Chain ID | | ∢ | ¥ | ¥ | V | A | | | | ¥ | В |
| PDB ID | | lekz | lekz | lekz | 1qu6 | 1qu6 | lstu | Istr | 1stu | 1b7f | lcvj |
| SEQ ID NO: | | 664 | 999 | 664 | 999 | 999 | 664 | 664 | 1 99 | 599 | 999 |

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|------------------|---|--|--|--|---|--|---|---|--|---|
| PDB annotation | PROTEIN-RNA COMPLEX, GENE REGULATION/RNA | GENE REGULATIONRNA POLY(A) BINDING ROCIENI I, PABE 1; RAN, PROTEIN-RINA COMPLEX, GENE REGULATION/RNA | RNA BINDING PROTEIN RNA- BINDING DOMAIN | STRUCTURAL PROTEIN PROTEIN C23; RNP, RBD, RRM, RNA BINDING DOMAIN, NUCLEOLUS | | RNA-BINDING DOMAIN RNA- BINDING DOMAIN, ALTERNATIVE SPLICING | RNA-BINDING PROTEIN SPLICING, U2 SNRNP, RBD, RNA-BINDING PROTEIN | COMPLEX (REDONCLEOPROTEINDNA) HNRNP A1, UP; COMPLEX (RIBONUCLEOPROTEINDNA), HETEROGENEOUS NUCLEAR 2 RIBONUCLEOPROTEIN A1 | TOXIN BINDING PROTEIN TWO DOMAINS: BETA PROPELLER AND ALPHAMETA FOLD | TOXIN BINDING PROTEIN TWO DOMAINS: BETA PROPELLER AND |
| Coumpound | D, E, F, G, H; RNA (5'- R(*AP*AP*AP*AP*AP*AP*AP *AP*AP*AP*A)-3'); CHAIN: M, N, O, P, Q, R, S, T; | POLYDENYLATE BINDING PROTEIN I; CHAIN: A, B, C, D, E, F, G, H; RNA (5'- R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP* | HU ANTIGEN C; CHAIN: A; | NUCLEOLIN RBDI; CHAIN: A; | RNA-BINDING PROTEIN SEX-LETHAL PROTEIN (C- TERMINUS, OR SECOND TERMINUS, OR SECOND 1SXL 3 (RBD-2), RESIDUES 199- 294 PLUS N-TERMINAL MED 1 SXL 4 (RMR, 17 STRUCTURES) 1SXL, 5 STRUCTURES) 1SXL, 5 | SEX-LETHAL PROTEIN; CHAIN: NULL; | SPLICING FACTOR U2AF 65 KD SUBUNIT; CHAIN: A; | HETEROGENEOUS NUCLEAR REGONUCLEOPROTEIN A1; CHAIN: A, 12-NUCLEOTIDE SINGLE-STRANDED TELOMETRIC DNA; CHAIN: B, | TOLB PROTEIN; CHAIN: A; | TOLB PROTEIN; CHAIN: A; |
| SeqFold score | | | | | | | | | | |
| PMF | | _ | 66.0 | 0.64 | 8.0 | 1 | - | - | 0.04 | 0.39 |
| Verify score | | 1.03 | 0.84 | 0.56 | 0.72 | 1.18 | 0.89 | 0.87 | 0.18 | 0.21 |
| PSI- BLAST | | 7.80E-11 | 1.30E-11 | 2.60E-11 | 1.30E-11 | 2.60E-11 | 7.80E-11 | 6.50E-11 | 0.0013 | 3.90E-06 |
| End AA | | 88 | 88 | 68 | 88 | | 88 | 88 | 269 | 217 |
| Start AA | | 01 | 6 | œ | 9 | 6 | 6 | ب | 126 | 11 |
| Chain ID | | н | ¥ | A | | | ¥ | ۷ | < _ | 4 |
| 808 O | | lcyj | 1d9a | 167 | 1sxl | 2sxl | 2u2f | 2up1 | lorz | lcrz |
| S e S | | 999 | 999 | 999 | 599 | 999 | 999 | 599 | 999 | 999 |

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|------------------|-----------------|---|---|--|---|--|---|---|---------------------------|
| PDB annotation | ALPHA/BETA FOLD | TRANSCRIPTION INHIBITOR BETA- PROPELLER | TRANSCRIPTION INHIBITOR BETA- PROPELLER | COMPLEX (GTP- BIDDINGTRANSDUCER, BETA1, TRANSDUCIN BETA SUBUNIT; GAMMA, TRANSDUCIN GAMMA SUBUNIT; COMPLEX (GTP- BINDINGTRANSDUCER), G PROTEIN, HETROSTRIMER 2 SIGNAL | COMPLEX (GTF- BINDINGTRANSDUCER) BETA1, TRANSDUCIN BETA SUBINIT; GAMMA, TRANSDUCIN GAMMA SUBDINT; COMPLEX (GTF- BINDINGTRANSDUCER), G PROTEIN, HETROSTRURE Z SIGNAL | COMPLEX (GTP- BIDDINGTRANSDUCER) BETA1, TRANSDUCIN BETA SUBUNIT: GAMMA, TRANSDUCIN GAMMA SUBUNIT: COMPLEX (GTP- BINDINGTRANSDUCER), G PROTEIN, HETEROTRINER 2 SIGNAL | COMPLEX (GTP- BIDDINGTRANSDUCER) BETA1, TRANSDUCTN BETA SUBINIT; GAMMA, TRANSDUCTN GAMMA SUBJUNT; COMPLEX (GTP- BINDINGTRANSDUCER), G PROTEIN, HETRORRIMER 2 SIGNAL | | TRANSFERASE DINUCLEOTIDE- |
| Coumpound | | TRANSCRIPTIONAL REPRESSOR TUPI; CHAIN: A, B, C; | TRANSCRIPTIONAL REPRESSOR TUP!; CHAIN: A, B, C; | GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT- BETA; CHAIN: B; GT- GAMMA; CHAIN: G; | GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT- BETA; CHAIN: B; GT- GAMMA; CHAIN: G; | GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT- BETA; CHAIN: B; GT- GAMMA; CHAIN: G; | GT-AI,PHA/GI-AI,PHA CHIMERA; CHAIN: A; GT- BETA; CHAIN: B; GT- GAMMA; CHAIN: G; | | NICOTINATE |
| SeqFold score | | | | _ | | 91.76 | | | |
| PMF | | 0.84 | 69.0 | - | -0.02 | | 0.8 | | -0.18 |
| Verify | | 0.2 | 0.24 | 0.59 | 0.27 | | 0.56 | | 0.52 |
| PSI- BLAST | | 1.80E-59 | 3.60E-69 | 7.20E-73 | 1.10E-57 | 1.10E-57 | 5.40E-56 | | 7.80E-14 |
| End | | 315 | 373 | 27.1 | 420 | 372 | 370 | | 194 |
| Start | | - | 30 | - | 118 | 29 | 71 | | 6 |
| Chain ID | | ¥ | 4 | м | м | Ф | В | | Ą |
| PDB CD | | lerj | lerj | 1got | lgot | 1got | 1got | | 1d0s |
| SEQ No. | | 999 | 999 | 999 | 999 | 999 | 999 | | 699 |

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|--------------------|--|---|--|-----------|---|-----------|---------------|-------------------------------|------------------------|-----------------------------|--------------------------|--------------------|---------------|------------|-----------------|-----------------------|-----------------------------|--------------------------|--------------------|---------------|-------------------|------------------------|-----------------------------|--------------------------|--------------------|--|--------------------------|-------------------------|----------------------------|---------------------|-------------------------|------------------------|------------------|--|
| PDB annotation | BINDING MOTIF, PHOSPHORIBOSYL TRANSFERASE | | TRANSCRIPTION HELIX-BUNDLE | | TRANSCRIPTION HELIX-BUNDLE | | | | | | | | | | | | | | | | | | | | | | TRANSCRIPTION REGULATION | PROTO-UNCOGENE, NUCLEAR | TRANSCRIPTION REGIT. ATION | | | | | LIGASE CBL, UBCH7, ZAP-70, E2, UBIQUITIN, E3, PHOSPHORYLATION, |
| Coumpound | MONONUCLEOTIDE:5,6- CHAIN: A; | | TRANSCRIPTION ELONGATION FACTOR S-II: | CHAIN: A; | TRANSCRIPTION FI ONGATION FACTOR S.II: | CHAIN: A; | TRANSCRIPTION | REGULATION TRANSCRIPTIONAL | FI ONGATION FACTOR SIL | (TFIIS, NUCLEIC-ACID 1TFI 3 | BINDING DOMAIN) (NMR, 12 | STRUCTURES) 1TFI 4 | TRANSCRIPTION | REGULATION | TRANSCRIPTIONAL | ELONGATION FACTOR SII | (TFIIS, NUCLEIC-ACID ITFI 3 | BINDING DOMAIN) (NMR, 12 | STRUCTURES) ITFI 4 | TRANSCRIPTION | TA ANSCRIPTION AT | FI ONGATION FACTOR SIL | (TFIIS, NUCLEIC-ACID 1TFI 3 | BINDING DOMAIN) (NMR, 12 | STRUCTURES) 1TFI 4 | The state of the s | TRANSCRIPTION FACTOR | PML; CFAIN: NOLL; | | VIRUS EQUINE HERPES | VIRUS-1 (C3HC4, OR RING | DOMAIN) ICHC 3 (NMR, I | SIRUCIURE) ICHC4 | SIGNAL TRANSDUCTION PROTEIN CBL; CHAIN: A; |
| SeqFold score | | | | | | | | | | | | | 75.24 | | | | | | | | | | | | | | | | | | | | | |
| PMF | | | 0.24 | | 0.21 | | _ | | | | | | | | | | | | | | | | | | | | 0.0 | | | 9.0 | | | | 0.45 |
| Verify | | | -0.43 | | -0.03 | | 0.24 | | | | | | | | | | | | | 0.26 | | | | | | ,,, | 6.65 | | | -0.48 | | | | -0.62 |
| PSI- BLAST | | | 1.00E-18 | | 1.10E-06 | | 1.80E-21 | | | | | | 1.30E-21 | | | | | | | 1.30E-2I | | | | | | 1 400 | 1.40E-06 | | | 1.80E-13 | | | | 9.10E-11 |
| End | | | 64 | | 09 | | 257 | | | | | | 257 | | | | | | | 257 | | | | | | 9,5 | 342 | | | 352 | | | 1 | 351 |
| Start AA | | | _ | | 4 | | 211 | | | | | | 212 | | | | | | | 212 | | | | | | 900 | 9 | | | 302 | | | - | /// |
| Chain The Chain | | | ٧ | | ¥ | | | | | | | .] | | | | | | | | | | | | | | | | | | | | | | V |
| 808 CO | | | 1000 | | leo0 | | JH1 | | | | | | Ŧ | _ | | | | | | Ħ | | | | | | | 1 por | | | 1chc | | | | ng. |
| S e S | | | 1/9 | | 1/9 | | 1/9 | | | | | | 671 | | | | | | | 1/9 | | | | | | 4 | 7/0 | | | 672 | _ | | Į | 7/9 |

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| PDB annotation | 2 TYROSINE KINASE, UBIQUITINATION, PROTEIN DEGRADATION, | LIGASE CBL, UBCH7, ZAP-70, E2, UBQUITN, B.; HOGSPHORYLATION, 2 TYROSINE KINASE, UBQUITINATION, PROTEIN DEGRADATION, | APOPTOSIS INHIBITOR OF APOPTOSIS (IAP), INMR STRUCTURE, BACULOVIRAL 2 IAP REPEAT (BIR), ZINC BINDING DOMAIN | DNA-BINDING PROTEIN V(D)J RECOMBINATION CATTU ATING PROTEIN I; RAGI, V(D)J RECOMBINATION, ANTIBODY, MAD, RING FINGER, 2 ZINC BINUCLEAR CLUSTER, ZINC FINGER, DNA- | DIA-BINDING PROTEIN V(D)J RECOMBINATION ACTIVATING PROTEIN I: RAGI, V(D)J RECOMBINATION, ANTIBODY, MAD, RING FINGER, Z ZINC BINUCILEAR CLUSTER, ZINC FINGER, DIA- BINDING PROTEIN | PEPTIDE SYNTHETASE GRSA; PEPTIDE SYNTHETASE, GRSA, ADENYLATE FORMING | PEPTIDE SYNTHETASE GRSA; PEPTIDE SYNTHETASE, GRSA, ADENYLATE FORMING | OXIDOREDUCTASE OXIDOREDUCTASE, MONOOXYGENASE, PHOTOPROTEIN, LUMINESCENCE |
| Coumpound | ZAP-70 PEPTIDE; CHAIN: B; UBIQUITIN-CONJUGATING ENZYME E12-18 KDA UBCH7; CHAIN: C; | SIGNAL TRANSDUCTION PROTEIN CBL; CHAIN: A; ZAP-70 PETTIDE; CHAIN: B; UBIQUITIN-CONJUGATING ENZYME BI2-18 KDA UBCH7: CHAIN: C; | INHIBITOR OF APOPTOSIS PROTEIN (2MIHB/C-IAP-1); CHAIN: A; | RAGI; CHAIN: NULL; | RAGI; CHAIN: NÜLL; | GRAMICIDIN SYNTHETASE 1; CHAIN: A, B; PHENYLALANINE; CHAIN: | GRAMICIDIN SYNTHETASE 1; CHAIN: A, B; PHENYLALANINE; CHAIN: C. D: | LUCIFERASE; CHAIN: NULL; |
| SeqFold score | | | | | | 158.05 | | 173.59 |
| PMF score | | 0.55 | 0.37 | 8:0 | 0.84 | | - | |
| Verify score | | -0.4 4 | -0.73 | 0.34 | -0.11 | | 9.0 | |
| PSI- BLAST | | 3.60E-13 | 0.0027 | 2.60E-09 | 7.20E-09 | 0 | 0 | 3.60E-93 |
| End | | 349 | 270 | 344 | 342 | 576 | 571 | 574 |
| Start | | 301 | 227 | | 302 | 24 | 39 | 22 |
| Chain TO | | ⋖ | ¥ | | | ∢ | 4 | |
| PDB CD | | Ifbv | 1qbh | Irmd | 1rmd | lam u | lam u | Ilci |
| S e S | | 672 | 672 | 7.59 | 219 | 673 | 673 | 673 |

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|-----------------|---|--|--|--|--|---|---|---|---|---|
| PDB annotation | OXIDOREDUCTASE OXIDOREDUCTASE, MONOOXYGENASE, PHOTOPROTEIN, LUMINESCENCE | TRANSCRIPTION REGULATION PROTO-ONCOGENE, NUCLEAR BODIES (PODS), LEUKEMIA, 2 TRANSCRIPTION REGULATION | TRANSCRIPTION REGULATION PROTO-ONCOGENE, NUCLEAR BODIES (PODS), LEUKEMIA, 2 TRANSCRIPTION REGULATION | TRANSCRIPTION REGULATION PROTO-ONCOGENE, NUCLEAR BODIES (PODS), LEUKEMIA, 2 TRANSCRIPTION PEGIT 4 TION | TRANSCRIPTION REGULATION PROTO-ONCOGENE, NUCLEAR BODIES (PODS), LEUKEMIA, 2 TRANSCRIPTION REGULATION | CELL MOTILITY PROTEIN MSP; CYTOSKELETAL PROTEIN, SPERM, CELL MOTILITY PROTEIN | CELL MOTILITY PROTEIN MSP; CYTOSKELETAL PROTEIN, SPERM, CELL MOTILITY PROTEIN | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGMIN ASSOCIATED 35 KDA PROTEIN, P35A, THREE HELIX BUNDLE | SCAFFOLD PROTEIN SCAFFOLD PROTEIN, PPZA, PHOSPHORYLATION, HEAT REPEAT | SMALL GTPASE KARYOPHERIN BETA, P95 SMALL GTPASE, NUCLEAR |
| Coumpound | LUCIFERASE; CHAIN: NULL; | TRANSCRIPTION FACTOR PML; CHAIN: NULL; | TRANSCRIPTION FACTOR PML; CHAIN: NULL; | TRANSCRIPTION FACTOR PML; CHAIN: NULL; | TRANSCRIPTION FACTOR PML; CHAIN: NULL; | MAJOR SPERM PROTEIN; CHAIN: A, B; | MAJOR SPERM PROTEIN; CHAIN: A, B; | SYNTAXIN-1A; CHAIN: A, B, C; | PROTEIN PHOSPHATASE PP2A; CHAIN: A, B; | RAN; CHAIN: A, C; IMPORTIN BETA SUBUNIT; |
| SeqFold | | | | | | | | | | |
| PMF | _ | 0.01 | 0.01 | 0.01 | 0.01 | 0.07 | 0.07 | -0.19 | -0.02 | 90.0 |
| Verify score | 0.77 | 0.21 | 0.21 | 0.21 | 0.21 | -0.05 | -0.05 | 0.12 | 0.16 | 0.02 |
| PSI- BLAST | 3.60E-93 | 0.0031 | 0.00054 | 0.0031 | 0.00054 | 7.80E-06 | 7.80E-06 | 7.80E-09 | 1.10E-51 | 5.40E-07 |
| End AA | 57.1 | 192 | 192 | 192 | 192 | 125 | 125 | 286 | 377 | 119 |
| Start | 36 | 144 | 144 | 144 | 144 | 34 | 34 | 165 | - | 22 |
| Chain | | | | | | V | V | A | A | В |
| PDB CI | :E | lbor | lbor | Ibor | Ibor | lmsp | lmsp | lez3 | 1b3u | libr |
| Š a Š | 673 | 675 | 675 | 919 | 919 | 619 | 089 | 189 | 682 | 682 |

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| PDB annotation | TRANSPORT RECEPTOR | NUCLEAR TRANSPORT PROTEIN COMPLEX HEAT REPEATS, NUCLEAR TRANSPORT PROTEIN COMPLEX | ARMADILLO REPEAT ARMADILLO REPEAT, BETA-CATENIN, CYTOSKELETON | POLYRIBONUCLEOTIDE TRANSTERASE DOLYNUCLEOTIDE PHOSPHORYLAS, GUANOSINE POLYRIBONUCLEOTIDE TRANSTERASE, ATF-CITP DIPHOSPHOTRANSFERASE, RNA PROCESSING, SNA DEGRADATION | POLYRIBONUCLEOTIDE TRANSTERASE DOLYNUCLEOTIDE TRANSTERASE OLYNUCLEOTIDE POLYRIBONUCLEOTIDE TRANSTERASE, ATP-GTP DIPHOSPHOTRANSTERASE, ZRAA PROCESSING, RNA DEGRADATION | | OXIDOREDUCTASE OXIDOREDUCTASE, OXYGENREDUCTASE, DIRON- CENTRE, 2 FLAVOROTEINS, LACTAMASE-FOLD | HYDROLASE METALLO-BETA- LACTAMASE, ANTIBIOTIC RESISTANCE, BINUCLEAR 2 ZINC, HYDROLASE | HYDROLASE METALLO-BETA- LACTAMASE, ANTIBIOTIC RESISTANCE, BINUCLEAR 2 ZINC, HYDROLASE | HYDROLASE HYDROLASE, BETA- LACTAMASE, ANTIBIOTIC, METALLOENZYME | REPLICATION PROTEIN A 32 DNA-BINDING PROTEIN RPA, OB- |
| Coumpound | CHAIN: B, D; | KARYOPHERIN BETA2; CHAIN: B; RAN; CHAIN: C; | BETA-CATENIN; CHAIN: NULL; | GUANOSINE PENTAPHOSPHATE SYNTHETASE; CHAIN: A; | GUANOSINE PENTAPHOSPHATE SYNTHETASE, CHAIN: A; | | RUBREDOXIN:OXYGEN OXIDOREDUCTASE; CHAIN: A, B | PENICILLINASE; CHAIN: A; | PENICILLINASE; CHAIN: A; | METALLO BETA- LACTAMASE II; CHAIN: A, B; | REPLICATION PROTEIN A 32 |
| SeqFold score | | | | | | | | | | | |
| PMF | | 0.07 | 0.09 | - | _ | | 90.0- | 0.04 | 60:0 | -0.05 | 0.23 |
| Verify score | | 0.11 | -0.18 | 0.55 | 0.62 | | 0.03 | 0.29 | -0.22 | 0.05 | 10.0 |
| PSI- BLAST | | 3.60E-37 | 1.30E-07 | 7.20E-58 | 7.20E-58 | | 3.60E-13 | 1.30E-18 | 0.00052 | 3.60E-10 | 3.60E-38 |
| End | | 400 | 363 | 273 | 273 | | 161 | 861 | 558 | 187 | 181 |
| Start AA | | 2 | 32 | | - | | 68 | 34 | 498 | 45 | 28 |
| Chain D | | В | | ⋖ | ¥ | | Ą | Ą | ٧ | ٧ | Ą |
| PDB DD | | Iqk | 3bct | 163h | 1e3p | | le5d | İsmi | lsml | 2bc2 | lquq |
| SEQ NO. ID | | 683 | 682 | 683 | 683 | | 684 | 684 | 684 | 684 | 989 |

| PDB annotation | FOLD, SSDNA-BINDING, DNA- BINDING PROTEIN | OXIDOREDUCTASE THIOREDOXIN M, | THIOREDOXIN | OXIDOREDUCTASE DIMER, THIOREDOXIN, X-RAY CRYSTALLOGRAPHY, OXIDOREDUCTASE | ELECTRON TRANSPORT ELECTRON TRANSPORT | TRYPAREDOXIN TRYX-1; TRYPAREDOXIN, CRITHIDIA | FASCICULATA, THIOREDOXIN, 2 TRYPANOSOME, ANOMALOUS | DISPERSION, UXIDATIVE STRESS, 3 OXIDOREDUCTASE | TRYPAREDOXIN TRYX-I; | TRYPAREDOXIN, CRITHIDIA EASCICIII ATA THIOPEDOXIN 2 | TRYPANOSOME, ANOMALOUS | DISPERSION, OXIDATIVE STRESS, 3 | PEROXIDASE 2-CVS | PEROXIREDOXIN, CALPROMOTIN | PEROXIDASE, PEROXIREDOXIN, SULPHINIC ACID, THIOREDOXIN | OXIDOREDUCTASE HEME-BINDING | THIOREDOXIN FOLD, | OXIDOREDUCTASE | ELECTRON TRANSPORT ALPHA/BETA OPEN-TWISTED PROTEIN, THIOL- | DISULFIDE | T7 DNA POLYMERASE, DNA REPLICATION, NUCLEOTIDYL 2 | TRANSFERASE, SEQUENCING, | THIOREDOXIN, PROCESSIVITY FACTOR, 3 COMPLEX |
|----------------|--|-------------------------------|-------------|--|---------------------------------------|---|---|--|------------------------|--|------------------------|---------------------------------|-------------------|----------------------------|---|-----------------------------|-------------------|----------------|--|-----------|--|--------------------------|---|
| Coumpound | KD SUBUNIT; CHAIN: A, C; REPLICATION PROTEIN A 14 KD SUBUNIT; CHAIN: B, D; | CHLOROPLAST | CHAIN: A; | THIOREDOXIN; CHAIN: NULL; | THIOREDOXIN M; CHAIN: A, B; | TRYPAREDOXIN-I; CHAIN: A; | | | TRYPAREDOXIN-I; CHAIN: | Ą; | | | HIMAN THIOREDOXIN | PEROXIDASE-B; CHAIN: A, | В, С, D, E, F, G, H, I, J, | THIOREDOXIN PEROXIDASE | Z, CRAIN: A, B; | | THIOREDOXIN; CHAIN: A; | | DNA POLYMERASE; CHAIN: A: THIOREDOXIN; CHAIN; B: | DNA; CHAIN: P, T; | |
| SeqFold | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.11 | | 60:0 | 10.0 | 0.18 | | | 0.34 | | | | -0.14 | | | 60:00 | | ; | | | 0.03 | | |
| Verify | | -0.28 | | 0.08 | -0.31 | -0.87 | | | 0.32 | | | | 90.0 | | | 0.1 | | 0,00 | 99:0- | | -0.36 | | |
| PSI- BLAST | | 3.60E-13 | | 3.60E-07 | 3.60E-11 | 5.40E-07 | | | 1.30E-12 | | | | 5.40E-40 | | | 1.60E-40 | | 1 200 | 1.30E-06 | | 1.60E-12 | | |
| End | | 147 | | 142 | 143 | 127 | | | 181 | | | | 233 | | | 210 | | 10. | <u> </u> | | 95 | | |
| Start AA | | 62 | | 90 | 09 | 70 | | | 75 | | | | 48 | | | 48 | | | % | | 75 | | |
| Chain | | < | | | ¥ | ¥ | | | Ą | | | | V | | | 4 | | | < | , | | | |
| PDB ID | | 1dby | | lerv | 1fb6 | 1qk8 | | | 14k8 | | | | 1 | · > | | 1qq2 | | 1 | ₽, | | d S | | |
| SEQ NO: | | 069 | | 069 | 069 | 069 | | | 069 | | | | 89 | | | 069 | | 9 | 060 | | 069 | | |

| PDB annotation | (HYDROLASE/ELECTRON TRANSPORT/DNA) | ÷ | | LIGASE CBI, UBCH7, ZAP-70, EZ, UBQUTTN, EZ, PORSPHORYLATION, 217YCOSINE KINASE, UBIQUITINATION, PROTEIN DEGRADATION, | LIGASE CBL, UBCH7, ZAP-70, E2, UBQUTIN, E3, PROSPHORYLATION, 2 17YROSINE KINASE, UBIQUITINATION, PROTEIN DEGRADATION, | DNA-BINDING PROTEIN V(DJ) RECOMBRIATION ACTIVATING PROTEIN I; RACI, V(DJ) RECOMBINATION, ANTIBODY, MAD, RING FINGER, 2 ZINC BINUCLEAR CLUSTER, ZINC FINGER, DNA- | DNA-BINDING PROTEIN V(DJ) RECOMBINATION ACTIVATING PROTEIN I; RACI, V(DJ) RECOMBINATION, ANTIBODY, MAD, RING PRICER, ZINC BINICLEAR CLUSTER, ZINC BINICLEAR BINDING PROTEIN | TRANSCRIPTION INHIBITOR BETA- PROPELLER | TRANSCRIPTION INHIBITOR BETA- |
|------------------|---------------------------------------|--|---|---|---|--|---|--|-------------------------------|
| Coumpound | | ELECTRON TRANSPORT THIOREDOXIN 2TRXA 2 2TRXA 3 | VIRUS EQUINE HERPES VIRUS-1 (C3HC4, OR RING DOMAIN) ICHC 3 (NMR, I STRUCTURE) ICHC 4 | SIGNAL TRANSDUCTION PROTEIN CBL; CHAIN: A; ZAP-70 PETTIDE; CHAIN: B; UBIQUITIN-CONJUGATING ENZYME E12-18 KDA UBCH7: CHAIN: C: | SIGNAL TRANSDÚCTION PROTEIN CBL; CHAIN: A; ZAP-70 PETTIDE; CHAIN: B; UBIQUITIN-CONJUGATING ENZYME E12-18 KDA UBCHT: CHAIN: C: | RAGI; CHAIN: NÚLL; | RAGI; CHAIN: NULL; | TRANSCRIPTIONAL REPRESSOR TUP1; CHAIN: A, | B, C; TRANSCRIPTIONAL |
| SeqFold score | | | | | | | | | |
| PMF | | 0.04 | 0.48 | 0.21 | 0.21 | 0.94 | 0.49 | 0.11 | 0.29 |
| Verify score | | 1.0- | -0.33 | -0.58 | -0.74 | -0.07 | -0.24 | 99.0 | 0.52 |
| PSI- BLAST | | 1.60E-12 | 7.20E-13 | 1.20E-10 | 1.80E-06 | 1.00E-13 | 5.40E-06 | 5.40E-42 | 9.00E-51 |
| End | | 150 | 363 | 363 | 368 | 363 | 368 | 307 | 369 |
| Start AA | | 62 | 318 | 298 | 319. | 297 | 319 | 4 | 71 |
| Chain 19 | | Ą | | ∢ | ∢ | | | ∢ | A |
| PDB ID | | 2trx | 1chc | 1fbv | 1fbv | Irmd | 1 гтр | 1erj | Eti |
| SEQ NO: | | 069 | 169 | 169 | 691 | 169 | 691 | 693 | 693 |

| PDB annotation | PROPELLER | COMPLEX (GTP. BINDING/TRANSDUCER) BETA1, TRANSDUCIN BETA SUBUNT; GAMMAI, TRANSDUCIN GAMMA SUBUNT; COMPLEX (GTP. BINDING/TRANSDUCER), G PROTEIN, HETROTRINER 2 SIGNAL. TRANSDUCTION | COMULEX (GTP. BINDING/TRANSDUCER, BETA1, TRANSDUCIN BETA SUBUNT; GAMAAI, TRANSDUCIN GAMAA SUBUNT; CONFLEX (GTP. BINDING/TRANSDUCER, G PROTEIN, HETROTRAMER 2 SIGNAL. TRANSDUCTION | COMPLEX (GTP. BUDDING/TRANSDICER,) BETA1, TRANSDICTR BETA SUBINIT, GAMMAI, TRANSDICTR GAMMA SUBUNIT; COMPLEX (GTP. BINDING/TRANSDICER), G PROTEIN, THETEROTRUMER 2 SIGNAL. | TOXIN BINDING PROTEIN TWO DOMAINS: BETA PROPELLER AND ALPHARETA FOI D | TRANSCRIPTION INHIBITOR BETA- PROPELLER | TRANSCRIPTION INHIBITOR BETA- PROPELLER | TRANSCRIPTION INHIBITOR BETA- PROPELLER | TRANSCRIPTION INHIBITOR BETA- PROPELLER |
|-----------------|------------------------------------|--|---|--|---|---|---|---|--|
| Coumpound | REPRESSOR TUP1; CHAIN: A, B, C; | GT-ALPHAGI-ALPHA CHIMERA, CHAIN: A; GT- BETA: CHAIN: B; GT- GAMMA; CHAIN: G; | GT-ALPHAGI-ALPHA CHIMERA, CHAIN: A; GT- BETA, CHAIN: B; GT- GAMMA; CHAIN: G; | GT-ALPHA/GI-ALPHA CHWERA, CHAIN: A; GT- BETA; CHAIN: B; GT- GAMMA; CHAIN: G; | TOLB PROTEIN; CHAIN: A; | TRANSCRIPTIONAL REPRESSOR TUPI; CHAIN: A, B. C: | TRANSCRIPTIONAL REPRESSOR TUPI; CHAIN: A, B, C; | TRANSCRIPTIONAL REPRESSOR TUPI; CHAIN: A, B. C: | TRANSCRIPTIONAL REPRESSOR TUP1; CHAIN: A, |
| SeqFold | | 70.14 | | | | | - | | |
| PMF | | | 0.16 | -0.17 | 0.29 | 0.94 | - | 6:0 | 91.0 |
| Verify score | | | 0.39 | 0.26 | 0.2 | 0.12 | 0.46 | 0.01 | 0.27 |
| PSI- BLAST | | 3.60E-57 | 3.60E-57 | 1.40E-36 | 9.00E-08 | 5.40E-78 | 1.80E-65 | 9.00E-57 | 1.40E-52 |
| End AA | | 376 | 370 | 304 | 377 | 416 | 313 | 442 | 224 |
| Start | | 28 | 39 | s | 133 | 801 | 18 | 195 | 5 |
| Chain ID | | В | щ | В | Ą | ∀ | ¥ | ∢ | Ą |
| FDB ED | | 1got | Igot | Igot | Icrz | lerj | lerj | lerj | lerj |
| SEQ NO: | | 693 | 693 | 693 | 694 | 694 | 694 | 694 | 694 |

| | _ | | · · · · · · · · · · · · · · · · · · · | Ţ | γ | |
|------------------|------|---|--|--|--|--|
| PDB annotation | | COMPLEX (GTP. BINDING/TRANSDUCER) BETA1, TRANSDUCIN BETA SUBUNIT; GAMAA1, TRANSDUCIN GAMMA SUBUNIT; COMPLEX (GTP- BINDING/TRANSDUCER), G PROTEIN, HETBROTRINGER, 2 SIGNAL | COMPLEX (GTP- BIDDINGTRANDUCER) BETAI, TRANSDUCTN BETA SUBINIT; GAMANI, TRANSDUCTN GAMMA SUBINIT; COMPLEX (GTP- BINDINGTRANSDUCER), G PROTEIN, HETEROTRINER 2 SIGNAL | COMPLEX (GTP- BINDINGTRANBUCER) BETAI, TRANSDUCIN BETA SUBUNIT; GAMAAI, TRANSDUCIN GAMMA SUBUNIT; COMPLEX (GTP- BINDINGTRANSDUCER), G PROTEIN, HETBROTRIMER 2 SIGNAL | COMPLEX (GTP- BIDDINGTRANSDUCER) BETAI, TRANSDUCIN BETA SUBUNIT: GAMAAI, TRANSDUCIN GAMMA SUBUNIT: COMPLEX (GTP- BIDDINGTRANSDUCER), G PROTEIN, HETEROSTRINER 2 SIGNAL | COMPLEX (GTP- BIDDINGTRANSDUCER) BETA1, TRANSDUCTN BETA SUBINIT; GAMAAI, TRANSDUCTN GAMMA SUBINIT; COMPLEX (GTP- BINDINGTRANSDUCER), G PROTEIN, HETROSTRANEX 2 SIGNAL. |
| Coumpound | B,C; | GT-ALPHAGI-ALPHA CHIMERA, CHAIN: A; GT- BETA, CHAIN: B; GT- GAMMA; CHAIN: G; | GT.ALPHA/GI.ALPHA CHINERA, CHANI. A; GT. BETA; CHANI: B; GT. GAMMA; CHANI: G; | GT-ALPHA/GI-ALPHA CHMERA, CHANI: A; GT- BETA; CHANI: B; GT- GAMMA; CHAIN: G; | GT-ALPHA/GI-ALPHA CHWIERA, CHARIN A; GT- BETA, CHAIN: B; GT- GAMMA; CHAIN: G; | GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT- BETA; CHAIN: B; GT- GAMMA; CHAIN: G; |
| SeqFold score | | | 105.8 | | | |
| PMF | | _ | | 0.21 | 0.22 | _ |
| Verify score | | 0.54 | | 0.26 | 0.36 | 0.69 |
| PSI- BLAST | | 5.40E-64 | 7.20E-81 | 3.60E-50 | 1.80E-53 | 7.20E-81 |
| End | | 393 | 353 | 443 | 267 | 353 |
| Start | | 103 | 12 | 061 | 4 | 95 |
| Chain ID | | В | ш | Ф | В | В |
| PDB ID | | 1got | lgot | 1got | Igot | lgot |
| SEQ NO: | | 694 | 694 | 694 | 694 | 694 |

| PDB annotation | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | | COMPLEX (ZINC FINGER/DNA) ZINC |
|-----------------|---|---|---|---|---|---|---|---|--|--------------------------------|
| Coumpound | QGSR ZINC FINGER PEFTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | QGSR ZINC FINGER PEPTIDE, CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE, CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B, C; | DNA-BINDING PROTEIN HUMAN ENHANCER. BINDING PROTEIN MBP.1 MUTANT WITH CYS II 1BBO 3 REPLACED BY ABU GLIABUJ (NMR, 60 STRUCTHER) 1BAO | DNA; CHAIN: A, B, D, E; |
| SeqFold | 84.99 | | | | | | | | · | |
| PMF | | _ | 0.03 | 0.81 | 69:0 | -0.17 | 69:0 | 0.39 | 0.09 | 0.45 |
| Verify score | | 0.18 | -0.13 | 0.03 | 0 | 0.13 | 0.14 | 1.0- | -0.35 | -0.09 |
| PSI- BLAST | 1.30E-31 | 3.60E-27 | 1.30E-31 | 7.20E-30 | 1.80E-28 | 5.40E-10 | 5.40E-28 | 3.60E-26 | 6.50E-11 | 1.80E-36 |
| End AA | 282 | 309 | 337 | 421 | 480 | 88 | 554 | 154 | 564 | 168 |
| Start | 200 | 228 | 228 | 341 | 397 | 40 | 484 | 74 | 514 | 101 |
| Chain ID | V V | 4 | ٧ | V | Y | ¥ | V | ¥ | | ပ |
| PDB ID | lalh | lalh | lalh | lalh | laih | lalh | lalh | lalh | ibbo | Ime |
| SEQ NO D | 169 | 269 | 269 | 697 | 269 | 697 | 697 | 697 | 697 | 269 |

| | | , | | | | , | | | |
|-----------------|---|--|--|--|--|--|--|--|--|
| PDB annotation | FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA |
| Coumpound | CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA: CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN: CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER |
| SeqFold | | | | | 97.32 | | | | |
| PMF score | | 0.16 | 0.8 | 1 | | 96.0 | 0.22 | 0.95 | 6:00 |
| Verify score | | -0.26 | 0.15 | 0.31 | | 0.27 | -0.23 | 0.21 | 0.41 |
| PSI- BLAST | | 1.30E-16 | 9.00E-35 | 5.40E-47 | 5.40E-47 | 3.60E-46 | 1.30E-33 | 3.60E-47 | 1.40E-49 |
| End | | 224 | 252 | 280 | 281 | 309 | 337 | 365 | 393 |
| Start AA | | 102 | 156 | 199 | | 227 | 227 | 283 | 312 |
| Chain ID | | ၁ | o_ | O | ပ | o | ပ | o | ၁ |
| PDB | ٧ | lme y | Jme y | Ime y | 1me y | Ime y | J me | Jme y | lme y |
| SEQ NO: | | 169 | 169 | 697 | 169 | 169 | | 269 | 169 |

| PDB annotation | INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX IZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX IZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX ZINC FINGERONA | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CNYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION PROTEIN DESIGN 2 |
|-----------------|---|--|--|--|--|--|--|--|---|
| Coumpound | PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN: CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA: CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; |
| SeqFold | | | | | | | | | |
| PMF | | 0.95 , | 0.88 | 90.04 | 0.62 | 0 | 0.86 | | 86:0 |
| Verify score | | 60:0 | 0 | 89.0- | 0.03 | 0.13 | 0.22 | 0.31 | 0.18 |
| PSI- BLAST | et- | 1.30E-48 | 1.80E-48 | 1.30E-21 | 3.60E.47 | 1.60E-35 | 3.60E-48 | 3.60E-50 | 1.10E-44 |
| End | | 422 | 451 | 208 | 480 | 126 | 808 | 536 | 557 |
| Start AA | | 340 | 368 | 368 | 396 | 42 | 425 | 455 | 483 |
| Chain | | υ | υ | ပ | ပ | ၁ | ပ | ပ | c |
| EDB DD | | Jme y | Imc y | lme y | Ime y | lme y | lme y | lme y | lme y |
| SEQ B B SS | | 697 | 169 | 269 | 697 | 169 | 169 | 269 | 269 |

| PDB annotation | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZNC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA INTERACTION PROTEIN DESIGN 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (TRANSCRIPTION PEGIT ATTIONIONA) TELLA : 62 CENE: | NMR TEITA PROTEIN DNA | TRANSCRIPTION FACTOR, 5S RNA 2 | GENE, DNA BINDING PROTEIN, ZINC | FINGER, COMPLEX 3 | COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX | PEGIII ATTOMONA) PNA | POLYMERASE III, 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX | (I KANSCKIP IION | REGULATION/DNA), RNA | INITIATION ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX | CIRANSCRIPTION | POLYMERASE III, 2 TRANSCRIPTION |
|------------------|--|--|--|--|---|--------------------------------|--|----------------------------|-------------------|---|-----------------------|--------------------------------|---------------------------------|-------------------|-------------------------|-------------------------|----------------------|---------------------------------|---------------------------------|------------------------|-------------------------|--------------------|----------------------|--------------------------------|-------------------------|-------------------------|--------------------|---------------------------------|
| Coumpound | | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER PROTEIN: CHAIN: CHEG | | | TRANSCRIPTION FACTOR | GENE: CHAIN: E. F. | | | | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; | CHAUN: B, C, E, F; | | | TFINA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | | | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | |
| SeqFold score | | | | | | | | | | | | | | | 107.54 | | | | | | | | | | | | | |
| PMF | | 0.58 | | 0.94 | | -0.13 | | | | 0.4 | | | | | | | | | | 0.92 | | | | | 0.75 | | | |
| Verify | | -0.2 | | 0.53 | | 0.3 | | | | | | | | | | | | | | 90.0 | | | | | -0.02 | | | |
| PSI- BLAST | | 1.80E-43 | | 5.40E-13 | | 1.10E-09 | | | | 1.10E-19 | | | | | 2.60E-50 | | | | | 3.60E-37 | | | | | 3.60E-34 | | | |
| End | | 154 | | 236 | | 8 | | | | 417 | _ | | | | 366 | | | | | 346 | | | | | 461 | | | |
| Start | | 13 | | 609 | | 71 | | _ | | 341 | | | | | 199 | | | | | 200 | | | | | 313 | | | |
| Chain | | ပ | | 5 | | g | | | | ∢ | | | | | A | | | | | ∢ | | | | | V | | | |
| EOS OO | | lme y | | lme y | | Ime | <u>`</u> | | | 9 | _ | | | | 146 | | | | | 碧 | | | | | 931 | | | |
| SEQ B B SE | | 169 | | . 169 | | 269 | | | | 697 | | | | | 697 | | | | | - 69 | | | | | 697 | | | |

| PDB annotation | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX | (INCANSCRIPTION) REGULATION/DNA), RNA | POLYMERASE III, 2 TRANSCRIPTION NITTATION ZNO FINGER PROTEIN | COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX | (TRANSCRIPTION | REGULATION/DNA), RNA | POLYMERASE III, 2 IRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX | (TRANSCRIPTION | REGULATION/DNA), KNA | NOT IMERASE III, 2 I KANSCRIPTION | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG I; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | (IKANSCKIPTION KEGULATION/DNA) | COMPLEX (TRANSCRIPTION PEGIT ATTOMONALYING YANG 1: | TRANSCRIPTION INITIATION | INITIATOR ELEMENT, YYL, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION |
|------------------|---------------------------------|---|---------------------------------------|--|-------------------------|-------------------------|--------------------|----------------------|---|-------------------------|-------------------------|--------------------|----------------------|-----------------------------------|------------------------|------------------------------|---------------------------|--------------------------------|-----------------------------|------------------------|--------------------------------|------------------------|------------------------------|---------------------------|--------------------------------|-----------------------------|------------------------|--------------------------------|---|--------------------------|--------------------------------|-----------------------------|------------------------|--------------------------------|------------------------|
| Coumpound | | TFIIIA; CHAIN: A, D; 58 RIBOSOMAL RNA GENE; | COMMIN: D, C, E, F; | | TEIIIA: CHAIN: A. D: 5S | RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | | | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | | YYI; CHAIN: C; ADENO- | INITIATOR EI EMENT DNA: | CHAIN: A. B: | î | | | YYI; CHAIN: C; ADENO- |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.23 | | | 0.72 | | | | | 0.01 | | | | | 69.0 | | | | | | | 0.51 | | | | | | | 0.95 | | | | | | 0.28 |
| Verify | | -0.13 | | | -0.02 | | | | | -0.39 | | | | | -0.35 | | | | | | | -0.29 | | | | | | | 9.18 | | | | | | 0.36 |
| PSI- BLAST | | 5.40E-36 | | | 1.80E-30 | | | | | 1.80E-27 | | | | | 1.80E-20 | | | | | | | 1.30E-39 | | | | | | | 1.305-31 | | | | | | 1.305-32 |
| End | | 489 | | | 558 | | | | | 233 | | | | | 224 | | | | | | | 338 | | | | | | | 337 | | | | | | 393 |
| Start | | 341 | | | 426 | | | | | 74 | | | | | 104 | | | | | | | 204 | | | | | | , , | 232 | | | | | | 760 |
| Chain | | A | | | V | | | | | ٧ | | | | | O | | | | | | | ပ | | | | | | ļ | <u>۔</u> ن | | | | | | 5 |
| PDB DD | | 911 | | | 110 | | | | | 146 | | | | | lubd | | | | | | | Inbd | | | | | | : | P P | | | | | | pgn |
| SEQ NO: | | 269 | | | 697 | | | | | 697 | | | | | 269 | | | | | | | 697 | | | | | | 100 | 2692 | | | | | į | 69/ |

| PDB annotation | REGULATION/DNA) YING-YANG 1; TRANCSHITON INTIATION, INTIATOR ELEMENT, TY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOOMITION, 3 COWELLEX (TRANSCHITON REGULATION/DNA) | COMPLEX (TRANSCRIPTION REQUILATIONDNA) YING-YANG I; TRANSCRIPTION INTITATION, MITIATIOR RELEMENT, YYI, ZINC 2 FINGER RECORNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REQUILT/IONDNA) YING-YANG I; TRANSCRIPTON INTLATION, INTLATOR ELEMENT, YY1, ZNC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULT/OND/NA YING-YANG I; TRANSCRIPTION INITIATION, INITIATIOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DINA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIOND/NA) | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-YANG I; TRANSCRIPTION INITATION, INITATION REMEMY, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOMITION, I COMPLEX RECOMITION, I COMPLEX | COMPLEX (TRANSCRIPTION REGULATIONNANA) YING-YANG I; TRANSCRIPTION INITIATION, INITIATIOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX |
|------------------|---|---|--|--|---|--|
| Coumpound | ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADBNO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C: ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; |
| SeqFold score | | | | | | 83.84 |
| PMF | | 0.7 | 0.99 | _ | 0.51 | |
| Verify score | | -0.3 | -0.03 | 11.0 | 0 | |
| PSI- BLAST | | 1,80 <u>E-33</u> | 9.00E-35 | 2.60E-28 | 3.60E-32 | 1.80E-34 |
| End AA | | 365 | 422 | 420 | 208 | 537 |
| Start AA | | | 320 | 345 | 404 | 427 |
| Chain 19 | | ပ | ၁ | ပ | ၁ | υ |
| 808 GI | | lubd | lubd | 1ubd | lubd | lubd |
| SEQ B G | | 697 | 269 | 697 | 269 | 697 |

| PDB annotation | COMPLEX (TRANSCRIPTION REGILATIONDNA) YING-YANG I; TRANSCRPTON INITATION, INITATIOR ELEMENT YYI, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION, SOMPLEX (TRANSCRIPTION REGILATIONDNA) | COMPLEX (TRANSCRIPTION REGULATONONA) YNG-YANG I; TRANSCRIPTON INITIATION, INITIATIOR BLEMENT YY1, ZINC 2 FINGER PROTEIN DIA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-YANG I; TRANSCRIPTON INITIATION, INITIATIOR ELEMENT, Y1, ZINC 2 FINGER PROTEIN DIA-PROTEIN RECOGNITION, SOMPLEX (TRANSCRIPTON REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULATIONDNA, YING-YANG I; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DINA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGILATIONNA) | TRANSCRIPTION REGULATION TRANSCRIPTION REGULATION, ADRI. ZINC FINGER, NAR | | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) |
|------------------|---|---|---|--|---|---|--|
| Coumpound | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INTIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED YIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | ADRI; CHAIN: NULL; | COMPLEX(TRANSCRIPTION REGULATION/DNA) TRAMTRACK PROTEIN (TWO ZINC-FINGER PEPTIDE) COMPLEXED WITH 2DRP 3 DNA 2DRP 4 | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; |
| SeqFold score | | | | | | | |
| PMF | 0.88 | 0.46 | 0.35 | 0.07 | 0.31 | -0.12 | 0.45 |
| Verify score | 0.06 | -0.05 | -0.25 | -0.45 | -0.15 | 0.26 | -0.08 |
| PSI- BLAST | 1.80E-34 | 3.60E-32 | 1,30E-26 | 1.30E-18 | 2.60E-14 | 1.30E-15 | 7.20E-26 |
| End | 536 | 558 | 154 | 253 | 980 | 264 | 279 |
| Start AA | 433 | 463 | 69 | 7.8 | 512 | 208 | 101 |
| Chain ID | ပ | ပ | ပ | ပ | | Ą | ٧ |
| PDB ID | Iubd | lubd | 1ubd | 1 ubd | 2adr | 2drp | 2gli |
| SEQ NO: | 697 | 697 | 697 | 697 | 269 | 169 | 269 |

| | | | | | | | | , | | | |
|-----------------|--|--|--|---|--|--|--|---|--|--|---------------------------|
| PDB annotation | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING , PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER. COMPLEX (DNA- BINDING PROTEINDNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINIDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDINA) | COMPLEX (DNA-BINDING |
| Coumpound | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLI1; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLJI; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLI1; |
| SeqFold | | | | | 89.2 | | | | | | |
| PMF | 66'0 | - | 0.25 | 66'0 | | 0.78 | 0.86 | 0.92 | 0.22 | 0.03 | 0.13 |
| Verify score | -0.17 | 0.14 | -0.24 | 90:00 | | -0.02 | 0.04 | 0.2 | 0.02 | -0.05 | -0.45 |
| PSI- BLAST | 6.50E-40 | 7.20E-28 | 5.20E-48 | 1.80E-32 | 5.20E-48 | 5.40E-35 | 3.60E-34 | 5.40E-33 | 1.60E-31 | 1.10E-24 | 3.90E-30 |
| End | 282 | 308 | 394 | 367 | 397 | 422 | 449 | 535 | 558 | 153 | 253 |
| Start AA | 102 | 198 | 200 | 235 | 255 | 292 | 320 | 404 | .433 | 99 | 77 |
| Chain ID | ¥ | ¥ | V | Ą | ¥ | ٧ | ۷. | ٧ | v | V | ٧ |
| 10 E | 2gli | . 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli |
| SEQ NO: | 269 | 169 | 169 | 269 | 169 | 169 | 697 | 169 | 169 | 169 | 697 |

| PDB annotation | PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIE; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN, | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION DYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | TD ANSEED ASE TP ANSEED ASE | KINASE, CALVIN CYCLE | TRANSFERASE TRANSFERASE, KINASE, CALVIN CYCLE | TRANSFERASE UPRTASE; TRANSFERASE, GLYCOSYLTRANSFERASE, UPRTASE | TRANSFERASE UPRTASE; TRANSFERASE, GLYCOSYLTRANSFERASE, UPRTASE | TRANSFERASE UPRTASE; TRANSFERASE, GLYCOSYLTRANSFERASE, UPRTASE | TRANSFERASE PANK; PROTEIN- |
|-----------------|--|---|--|---|---|---|--|--|-----------------------------|----------------------|--|--|--|--|----------------------------|
| Coumpound | CHAIN: A; DNA; CHAIN: C, D; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | PUCEPUCPIEI OF IN A CE. | CHAIN: NULL; | PHOSPHORIBULOKINASE; CHAIN: NULL; | URACIL PHOSPHORIBOSYLTRANSFE RASE; CHAIN: D, C, B, A; | URACIL PHOSPHORIBOSYLTRANSFE RASE; CHAIN; D. C. B. A; | URACIL PHOSPHORIBOSYLTRANSFE RASE: CHAIN: D. C. B. A: | PANTOTHENATE KINASE; |
| SeqFold | | | 62.4 | | 64.18 | | | | | | 6.99 | 191.89 | | | |
| PMF | | 0.63 | | -0.12 | | 91.0 | 0.04 | 0.01 | 90 | 0:0 | | | _ | _ | 96'0 |
| Verify score | | -0.1 | | 9.04 | | -0.03 | -0.22 | 80.0- | 0.17 | 0.17 | | | 0.84 | 0.76 | 0.43 |
| PSI- BLAST | | 7.20E-32 | 7.20E-32 | 1.40E-34 | 1.80E-32 | 1.80E-32 | 1.30E-06 | 1.30E-08 | 1 30E-13 | 1.700 | 1.30E-13 | 2.60E-73 | 3.60E-44 | 2.60E-73 | 1.80E-35 |
| End | | 302 | 300 | 178 | 302 | 302 | 62 | 182 | 186 | 9 | 366 | 532 | 532 | 232 | 294 |
| Start | | 101 | 74 | 9 | 02 | 74 | 23 | 74 | 128 | 2 | 95 | 306 | 322 | 324 | 75 |
| Chain ID | | ¥ | ¥ | 4 | ٧ | A | | | ĺ | | | Д | Д | Д | A |
| PDB ID | | 1edh | ledh | lncj | Incj | 1ncj | 1suh | 1suh | 197 | | 1a7j | 1543 | 1643 | 1643 | lesm |
| S e S | | 869 | 869 | 869 | 869 | 869 | 869 | 869 | Ę | į | 101 | 701 | 101 | 101 | 701 |

| | _ | | | | | _ | | | γ | | | | |
|------------------|--------------------|---|---|---|--|---|---|---|--|--|---|--|---|
| PDB annotation | INHIBITOR COMPLEX | TRANSFERASE PANK; PROTEIN- INHIBITOR COMPLEX | | PHOSPHOTRANSFERASE ADK; PHOSPHOTRANSFERASE, ZINC FINGER | KINASE KINASE, PHOSPHOTRANSFERASE | | CHAPERONE HSP40; CHAPERONE, HEAT SHOCK, PROTEIN FOLDING, DNAK | CHAPERONE HSP40; CHAPERONE, HEAT SHOCK, PROTEIN FOLDING, DNAK | GENE REGULATIONRNA POLY(A) BINDING BYOTEN I, PABP I; RRM, PROTEIN-RIA COMPLEX, GENE REGULATIONRNA | GENE REGULATIONRNA POLY(A) BINDING PROTEIN I, PABE 1; RRM, PROTEIN-RIA COMPLEX, GENE REGULATIONRNA | GENE REGULATIONRNA POLY(A) BINDING BYOTEIN I, PABP 1; RRM, PROTEIN-RIA COMPLEX, GENE REGULATIONRNA | RNA BINDING PROTEIN RNA- BINDING DOMAIN | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGMIN ASSOCIATED 35 |
| Coumpound | CHAIN: A, B, C, D; | PANTOTHENATE KINASE; CHAIN: A, B, C, D; | TRANSFERASE URIDYLATE KINASE (E.C.2.7.4) COMPLEXED WITH ADP AND AMP 11K7 3 | ADENYLATE KINASE; CHAIN: NULL; | THYMDYLATE KINASE; CHAIN: A, B, C, D, E, F, G, H; | | DNAJ; CHAIN: NULL; | DNAJ; CHAIN: NULL; | POLYDENYLATE BINDING PROTEIN 1; CHAIN: A, B, C, D, E, F, G, H; RNA (5'- R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP* | POLYDENYLATE BINDING PROTEIN 1; CHAIN: A, B, C, D, E, F, G, H; RNA (5'- R(*AP*AP*AP*AP*AP*AP*AP *AP*AP*AP*AP; CHAIN: AN N, O, P, O, R, S, T; | POLYDENYLATE BINDING PROTEIN I; CHAIN: A, B, C, D, B, F, G, H; RNA (5'. R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP* | HU ANTIGEN C; CHAIN: A; | SYNTAXIN-1A; CHAIN: A, B, C; |
| SeqFold | | | | | | | 54.61 | | | | | | |
| PMF score | | 66'0 | 0.54 | 0.21 | 0.03 | | | 0.52 | 69:0 | 0.46 | 0.46 | 0.93 | -0.13 |
| Verify | | 0.55 | 0.19 | -0.33 | -0.38 | | | 0.52 | 0.07 | 0.13 | 0.03 | 0.15 | 0.14 |
| PSI- BLAST | | 6.50E-67 | 1.20E-15 | 0.0078 | 1.30E-23 | | 1.30E-31 | 1.30E-31 | 3.60E-14 | 1.80E-12 | 1.80E-12 | 1.80E-12 | 1.30E-09 |
| End AA | | 303 | 302 | 302 | 303 | | 84 | 84 | 255 | 259 | 259 | 251 | 186 |
| Start AA | | 16 | \$ | 105 | 96 | | 8 | 6 | 182 | 781 | 182 | 185 | 11 |
| Chain ID | | ¥ | | | υ U | | | | ¥ | CL. | н | ٧ | ٧ |
| PDB | | lesm | lukz | 1zin | 3tmk | | 1bq0 | 1bq0 | 1cvj | 1cvj | lcvj | 1d8z | lez3 |
| SEQ ID NO: | | 101 | 101 | 701 | 101 | | 702 | 702 | 702 | 702 | 702 | 702 | 702 |

| | | | | | | | _ | | | | |
|------------------|--|---|--|---|---|---|--|--|---|--|------------------------|
| PDB annotation | KDA PROTEIN, P35A, THREE HELIX BUNDLE | NUCLEAR RROTEIN HETREOGENEOUS NUCLEAR RIBONUCLEOPROTEIN A1, NUCLEAR PROTEIN, HARNP, RBD, RRM, RNP, RNA BINDING, 2 RIBONUCLEOPROTEIN | RNA BINDING PROTEIN RNA- BINDING DOMAIN | MOLECULAR CHAPERONE HDJ-1; MOLECULAR CHAPERONE | MOLECULAR CHAPERONE HDI-I; MOLECULAR CHAPERONE | MOLECULAR CHAPERONE HDJ-1; MOLECULAR CHAPERONE | RNA BINDING PROTEIN RNA- BINDING DOMAIN | COMPLEX (RIBONUCLEOPROTEINDNA) HNRNP AI, UP; COMPLEX (RIBONUCLEOPROTEINDNA), HETEROGENEOUS NUCLEAR 2 RIBONUCLEOPROTEIN A1 | COMPLEX (RIBONUCLEOPROTEINDNA) HIRRIP AI, UP; COMPLEX (RIBONUCLEOPROTEINDNA), HETEROGENEOUS NUCLEAR 2 RIBONUCLEOPROTEIN AI | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGIMIN ASSOCIATED 35 KDA PROTEIN, P35A, THREE HELIX BUNDLE | COMPLEX (TRANSCRIPTION |
| Coumpound | | HNRNP A1; CHAIN: NULL; | HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN DO; CHAIN: A; | HUMAN HSP40; CHAIN: NULL; | HUMAN HSP40; CHAIN: NULL; | HUMAN HSP40; CHAIN: NULL; | MUSASHII; CHAIN: A; | HETEROGENEOUS NUCLEAR REGONICLEOPROTEIN A1; CHAIN: A, 12-NUCLEOTIDE SINGLE-STRANDED TELOMETRIC DNA; CHAIN: B; | HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN AI; CHAIN: A; 12-NUCLEOTIDE SINGLE-STRANDED TELOMETRIC DIA; B; | SYNTAXIN-1A; CHAIN: A, B, C; | GA BINDING PROTEIN |
| SeqFold score | | | | | 56.45 | | | | | | 63.45 |
| PMF | | 0.19 | 0.51 | _ | | 0.47 | 0.18 | 0 | 0.05 | 0.11 | |
| Verify | · | 0.33 | 0.12 | 0.57 | | 0.0 | 0.42 | 0.16 | -0.11 | 0.15 | |
| PSI- BLAST | | 1.30E-22 | 5.40E-16 | 2.60E-19 | 1.80E-28 | 1.80E-28 | 7.20E-17 | 5.40E-26 | 1.30E-18 | 6.50E-06 | 1.80E-36 |
| End | | 249 | 249 | 78 | 84 | . 48 | 249 | 255 | 259 | 575 | 292 |
| Start AA | | 182 | 182 | = | œ | ∞ | 182 | 91 | 182 | 468 | 137 |
| Chain | | | 4 | | | | A | ∀ | ∢ | 4 | В |
| සු ය | | lhal | 1hd1 | 1hdj | 1hdj | .ipqi | 2mss | 2up1 | 2up1 | 1ez3 | lawc |
| SEQ No. | | 702 | 702 | 702 | 702 | 702 | 702 | 702 | 702 | 705 | 902 |

| PDB annotation | REGULATION/DNA) GÁBPALPHA; GABPBETA; COMPLEX (TRANSCRIPTION REGULATION/DNA, DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKTYRN REPEATS, TRANSCRIPTION 3 FÁCTOR | COMPLEX (TRANSCRIPTION REGULATION/DAY) OABALPHA; GABPERTAL; COMPLEX (TRANSCRIPTION TREGULATION/DAY) DIA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION 3 PACTOR | COMPLIX (TRANSCRIPTION REGULATIONDINA) OABPALPHA; GABPBETA!: COMPLEX (TRANSCRIPTION REGULATION/DIA), DIA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, AINXTRIN REPEATS, TRANSCRIPTION 3 PACTOR. | COMPLEX (TRANSCRIPTION REQUIL/TROUNDAY) OBBALPHA; GABBERTA!; COMPLEX (TRANSCRIPTION TREGUIL/ATTON/DAY) DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION 3 PACTOR. | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR |
|------------------|---|---|---|---|--|--|--|------------------------|
| Coumpound | ALPHA; CHAIN: A; GA BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN ALPHA, CHAIN: A; GA BINDING PROTEIN BETA I; CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN ALPHA; CHAIN: A; GA BINDING PROTEIN BETA I; CHAIN: B; DNA; CHAIN: D; E; | GA BINDING PROTEIN ALPHA, CHRINE, A; GA BINDING PROTEIN BETA I; CHAIN: B; DNA; CHAIN: D; E; | P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | P19INK4D CDK4/6 |
| SeqFold score | | | | | 62.42 | | | |
| PMF | | - | 1 | 0.86 | | 1 | _ | -0.14 |
| Verify score | | 0.84 | 0.49 | 0.51 | | 0.85 | 0.72 | 0.03 |
| PSI- BLAST | | 1.30E-30 | 1.80E-36 | 7.20E-33 | 3.60E-31 | 3.60E-31 | 9.00E-31 | 3.60E-27 |
| End | | 273 | 323 | 351 | 298 | 293 | 320 | 224 |
| Start AA | | 169 | | 209 | 144 | 145 | 178 | 57 |
| Chain D | | æ | g | д | | | | 1 |
| 808 E1 | - | Iawc | lawc | lawc | 3PqI | 1bd8 | 8P91 | 1bd8 |
| S a S | | 706 | 902 | 706 | 902 | 902 | 902 | 90/ |

| PDB annotation | SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | COMPLEX (INHIBITOR PROTEINGARS) PROTEINGARS) INHIBITOR PROTEIN (CYCLIA-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHANEST, COMPLEX (INHIBITOR PROTEIN/KINASE) | COMPLEX (INHIBITOR PROTEINAVIASE) NHHBITOR PROTEIN, CYCLIA-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHADELT, COMPLEX (INHIBITOR PROTEIN/KINASE) | COMPLEX (INHIBITOR PROTEIN/KIASE) NHBITOR PROTEIN, CYCLA-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHADETA, COMPLEX (INHIBITOR PROTEIN/KINASE) | COMPLEX (INHIBITOR PROTEINGARS) PROTEINGKARSE) INHIBITOR PROTEIN, CYCLP, DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHANEST, A COMPLEX (INHIBITOR PROTEIN/KINASE) | HORMONE/GROWTH FACTOR P18- INK4C; CELL CYCLE INHBITOR, P18INK4C; UNOMS, SUPPRESSOR, CYCLIN-12 DEPENDENT KINASE, HORMONE/GROWTH FACTOR | HORMONE/GROWTH FACTOR P18- INK4C; CELL CYCLE INHBITOR, P18INK4C; TUMOR, SUPPRESSOR, CYCLIN- 2 DEPENDENT KINASE, HORMONE/GROWTH FACTOR | SIGNALING PROTEIN HELIX-TURN- HELIX, ANKYRIN REPEAT | CELL CYCLE INHIBITOR P18- INK4C(INK6); CELL CYCLE |
|-----------------|--|--|--|---|--|---|---|--|--|
| Coumpound | INHIBITOR; CHAIN: NULL; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; PI9INK4D; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; PI9INK4D; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6, CHAIN: A; P19INKAD; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A; | CYCLIN-DEPENDENT KINASE 4 INHIBITOR B; CHAIN: A; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; |
| SeqFold | | 63.41 | | | | 74.38 | | | 68.42 |
| PMF | | | _ | 96.0 | | | 0.95 | _ | |
| Verify score | | | 0.71 | 59.0 | 0.24 | | 19:0 | 0.55 | |
| PSI- BLAST | | 1.10E-30 | 1.80E-30 | 1.10E-30 | 3.60E-26 | 9.00E-34 | 9.00E-34 | 1.305-28 | 5.40E-33 |
| End | | 297 | 293 | 315 | 224 | 302 | 329 | 273 | 296 |
| Start AA | | 144 | 145 | 178 | 57 | 134 | 5/1 | 171 | 138 |
| Chain D. | | В | m · | В | В | ₹ . | ∢ | ¥ | ٧ |
| EDB EDB | | 1bk | 1blx | 1bk | 1bk | 1bu9 | 1bu9 | 1d9s | 1ih |
| ğa ÿ | | 902 | 706 | 706 | 902 | 706 | 902 | 706 | 706 |

| PDB annotation | INHIBITOR, P18-INK4C(INK6), ANKYRIN REPEAT, 2 CDK 4/6 INHIBITOR | CELL CYCLE INHIBITOR P18- DNRAC(INK 6); CELL CYCLE INHIBITOR, P18-DRAC(INK 6), MNYRIN REPEAT, 2 CDK 4/6 INHIBITOR | TRANSCRIPTION FACTOR P65, P50D; TRANSCRIPTION FACTOR, IKBNFKB COMPLEX | TRANSCRIPTION FACTOR P65: P50D; TRANSCRIPTION FACTOR, IKBNFKB COMPLEX | ANK-REPEAT MYOTROPHIN, ACETYLATION, NMR. ANK-REPEAT | ANK-REPEAT MYOTROPHIN, ACETYLATION, NMR. ANK-REPEAT | COMPLEX (TRANSCRIPTION REG/ANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT) ANKYRN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION REGIANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT) ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION REGIANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT) ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION REGIANK REPEAT) COMPLEX (TRANSCRIPTION REGULATIONANK REPEAT) ANKYRN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION REG/ANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT) ANKYRIN 2 REPEAT HE 1X | COMPLEX (TRANSCRIPTION |
|------------------|---|---|---|---|---|---|--|---|---|---|---|---------------------------|
| Coumpound | CHAIN: A, B; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA; CHAIN: D; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA; CHAIN: D; | MYOTROPHIN; CHAIN: NULL | MYOTROPHIN; CHAIN: NULL | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E, P: | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E, F: | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E, F: | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E. F: | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E. F. | NF-KAPPA-B P65; CHAIN: A, |
| SeqFold score | | | | 74.07 | 66.09 | | | | | | | 71.81 |
| PMF | | 0.99 | 9.0 | | | _ | -0.06 | _ | 0.46 | 0.18 | 0.98 | |
| Verify score | | 0.88 | 0.26 | | | 0.32 | 0 | 69:0 | 0.55 | 0.18 | 0.26 | |
| PSI- BLAST | | 5.40E-33 | 7.20E-41 | 7.20E-41 | 2.60E-32 | 2.60E-32 | 1.10E-36 | 5.40E-36 | 1.80E-34 | 3.60E-27 | 3.60E-41 | 3.60E-41 |
| End | | 328 | 290 | 307 | 288 | 287 | 208 | 310 | 341 | 414 | 290 | 303 |
| Start AA | | 175 | 82 | 56 | 691 | 172 | 12 | 136 | 691 | 204 | | 95 |
| Chain | | < | Ω | О | | | ш | ш | В | ជ | ы | Е |
| 808 CI | | lib 1 | liku | lika | lmy 0 | lmy | ful | gu! | lnfi | <u> </u> | Infi | Infi |
| SEQ NO: | | 902 | 902 | 902 | 90/ | 902 | 902 | 90/ | 902 | 706 | 902 | 90/ |

| | | · | _ | | | | | | | | |
|------------------|---|--|---|--|--|---|--|--|--|---------------------------------------|---|
| PDB annotation | REG/ANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX | COMPLEX (ANT). ONCOGENEANKYRIN REPEATS) PASSEZ, ANKYRIN REPEATS, 8H, 934, TUMOR SUPPRESSOR, MULTIGENE 2 FAMILY, NUCLEAR PROTEIN, PHOSPHORYLATION, DISEASE MUTATION, 3 POLYMORPHISM, COMPLEX (ANT). | | CALCUM-BINDING PROTEIN CALSEQUESTRIN, CALCUM-BINDING PROTEIN, SARCOPLASMIC 2 RETICULUM, RABBIT SKELETAL MUSCLE | CALCIUM-BINDING PROTEIN CALSEQUESTRIN, CALCIUM-BINDING PROTEIN, SARCOPLASMIC 2 RETICULUM, RABBIT SKELETAL MUSCLE | ELECTRON TRANSPORT ELECTRON TRANSPORT, REDOX-ACTIVE CENTER, ISOMERASE, 2 ENDOPLASMIC RETICULUM | OXIDOREDUCTASE THIOREDOXIN M, THIOREDOXIN CH2, CHLOROPLASTIC THIOREDOXIN | OXIDOREDUCTASE THIOREDOXIN M, THIOREDOXIN CH2, CHLOROPLASTIC THIOREDOXIN | OXIDOREDUCTASE DIMER, THIOREDOXIN, X-RAY CRYSTALLOGRAPHY, OXIDOREDUCTASE | ELECTRON TRANSPORT ELECTRON TRANSPORT | ELECTRON TRANSPORT ELECTRON TRANSPORT, REDOX-ACTIVE |
| Coumpound | C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E, F; | P33, CHAIN: A; 33BP2, CHAIN: B; | | CALSEQUESTRIN, CHAIN: NULL | CALSEQUESTRIN; CHAIN: NULL | PROTEIN DISULFIDE ISOMERASE; CHAIN: NULL; | CHLOROPLAST THIOREDOXIN M CH2; CHAIN: A: | CHLOROPLAST THIOREDOXIN M CH2; CHAIN: A; | THIOREDOXIN; CHAIN: NULL; | THIOREDOXIN M; CHAIN: A, B; | PROTEIN DISULFIDE ISOMERASE; CHAIN: NULL; |
| SeqFold score | | 75.09 | | 87.98 | | | 52.47 | | | | 82.03 |
| PMF score | | | | | 96:0 | 0.07 | | 0.95 | 86.0 | _ | |
| Verify score | | | | | 0.15 | -0:03 | | 0.3 | 0.54 | 0.81 | |
| PSI- BLAST | | 1.80E-25 | | 5.40E-42 | 5.40E-42 | 1.60E-13 | 5.40E-24 | 5.40E-24 | 1.10E-23 | 9.00E-25 | 1.10E-31 |
| End | | 362 | ì | 336 | 332 | 239 | 131 | 131 | 128 | 130 | 134 |
| Start AA | | 170 | , | 2 | 20 | 133 | 23 | 30 | 41 | 27 | 20 |
| Chain ID | | m | | | | | ∢ | Ą | | ¥ | |
| PDB ID | | lycs | | la8y | 1a8y | 16jx | Idby | ldby | lerv | 1£96 | lme k |
| SEQ No. id | | 706 | 1 | 6 | 60/ | 602 | 90 | 602 | 709 | 709 | 402 |

| PDB annotation | CENTER, ISOMERASE, 2 ENDOPLASMIC RETICULUM | ELECTRON TRANSPORT ELECTRON TRANSPORT, REDOX-ACTIVE CENTER, ISOMERASE, 2 ENDOPLASMIC RETICULUM | ELECTRON TRANSPORT ALPHABETA OPEN-TWISTED PROTEIN, THIOL- DISULFIDE | | TT DNA POLYNERASE DNA REPLICATION, NUCLEOTIDYL 2 TRANSFERASE, SEQUENCING, TRANSFERASE, SEQUENCING, THOREDOXIN, PROCESSIVITY FACTOR, 3 COMPLEX HYDROLASSELECTRON TRANSPORTIONAL | ELECTRON TRANSPORT THIOREDOXIN 2: 1THX 7 OXIDO- REDUCTASE ITHX 16 | ELECTRON TRANSPORT THIOREDOXIN 2; ITHX 7 OXIDO- REDUCTASE ITHX 16 | ELECTRON TRANSPORT HTRX, HCHI, CHI, OXIDOREDUCTASE, ELECTRON TRANSPORT | | | | DNA INTEGRATION |
|------------------|---|---|---|--|--|---|---|--|--|--|----|---|
| Coumpound | | PROTEIN DISULFIDE ISOMERASE; CHAIN: NULL; | THIOREDOXIN; CHAIN: A; | DNA POLYMERASE; CHAIN: A; THIOREDOXIN; CHAIN: B; DNA; CHAIN: B, T; | DNA POLYMERASE; CHAIN: A; THIOREDOXIN; CHAIN: B; DNA; CHAIN: P, T; | THIOREDOXIN; 1THX 5 CHAIN: NULL; 1THX 6 | THIOREDOXIN; 1THX 5 CHAIN: NULL; 1THX 6 | THIOREDOXIN H; CHAIN: NULL; | ELECTRON TRANSPORT THIOREDOXIN 2TRXA 2 2TRXA 3 | ELECTRON TRANSPORT THIOREDOXIN 2TRXA 2 2TRXA 3 | | AVIAN SARCOMA VIRUS INTEGRASE; IASU 7 CHAIN: |
| SeqFold score | | | | 60.72 | | 55.88 | | | 62.2 | | | |
| PMF | | 86:0 | _ | | _ | | 1 | 99'0 | | 1 | | 0.39 |
| Verify | | 0.43 | 0.62 | | 0.39 | | 0.75 | 0.33 | | 0.39 | | -0.13 |
| PSI- BLAST | | 1.10E-31 | 3.60E-24 | 1.60E-24 | 1.60E-24 | 9.10E-22 | 9.10E-22 | 9.00E-23 | 5.40E-25 | 5.40E-25 | | 1.80E-25 |
| End | | 133 | 130 | 128 | 130 | 131 | 125 | 129 | 131 | 130 | | 283 |
| Start AA | | 21 | 30 | 92 | . 72 | 24 | 32 | 25 | 24 | 25 | 95 | 98 |
| Chain 1D | | | ¥ | æ | B | | | | ٧ | ٧ | | |
| PDB ID | | r Inc | ıg * | d/31 | lt7p | Ithx | Ithx | Itof | 2trx | 2trx | | lasu |
| SEQ NO ID | | 902 | 709 | 907 | 709 | 709 | 709 | 709 | 709 | 709 | 1 | 2 |

| PDB annotation | | TRANSFERASE DNA INTEGRATION | TRASFERASE DNA INTEGRATION, TRASFERASE | DNA INTEGRATION DNA | INTEGRATION, AIDS, POLYPROTEIN, | HYDROLASE, 2 ENDONUCLEASE, | POLYNUCLEOTIDYL TRANSFERASE, | DNA BINDING 3 (VIRAL) | TRANSFERASE INTEGRASE, ROUS | SARCOMA VIRUS, HIV, X-RAY | CRYSIALLOGRAPHY, 2 PROLEIN | VIRIS/VIRAL PROTEIN INTEGRASE | ROUS SARCOMA VIRUS, HIV, X-RAY | CRYSTALLOGRAPHY 2 VIRTIS/VIRAL | PROTEIN | TRANSFERASE MIXED BETA-SHEET | SURROUNDED BY ALPHA-HELICES | VIRUS/VIRAL PROTEIN HIV-1 | INTEGRASE, POLYNUCLEOTIDYL | TRANSFERASE, DNA-BINDING 2 | PROTEIN, DD35E | HYDROLASE DNA INTEGRATION, | INTEGRASE, HIV, HYDROLASE, | ASPARTYL 2 PROTEASE, | TOUROGERUSE | ANTI-ONCOGENE CELL CYCLE, ANTI- | ONCOGENE, REPEAT, ANK REPEAT | ANTI-ONCOGENE CELL CYCLE, ANTI- | ONCOGENE, REPEAT, ANK REPEAT | COMPLEX (TRANSCRIPTION | CADDETA1: COMMITTY | CTR ANSCRIPTION | REGULATION/DNA-BINDING 2 | NUCLEAR PROTEIN, ETS DOMAIN, | ANKYRIN REPEATS, TRANSCRIPTION | COMPLEX (TRANSCRIPTION | |
|------------------|--------------|-----------------------------|---|----------------------------|---------------------------------|----------------------------|------------------------------|-----------------------|-----------------------------|---------------------------|----------------------------|-------------------------------|--------------------------------|--------------------------------|---------|------------------------------|-----------------------------|---------------------------|----------------------------|----------------------------|----------------|----------------------------|----------------------------|----------------------|-------------|---------------------------------|------------------------------|---------------------------------|------------------------------|------------------------|-------------------------|-----------------------------|--------------------------|------------------------------|--------------------------------|------------------------|--|
| Coumpound | NULL; 1ASU 8 | INTEGRASE; CHAIN: A; | INTEGRASE; CHAIN: A; | INTEGRASE; CHAIN: A, B, C; | | | | | INTEGRASE; CHAIN: A, B, C, | Ď; | | RSV INTEGRASE: CHAIN: A | B; | | | AVIAN SARCOMA VIRUS | INTEGRASE; CHAIN: A; | POL POLYPROTEIN; CHAIN: | A, B; | | | HIV-1 INTEGRASE; CHAIN: | A, B, C; | | | TUMOR SUPPRESSOR | PI6INK4A; CHAIN: NULL; | TUMOR SUPPRESSOR | PI6INK4A; CHAIN: NULL; | GA BINDING PROTEIN | PINDING PROTEIN BETA 1. | CHAIN: B: DNA: CHAIN: D. E. | | | | GA BINDING PROTEIN | |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | 72.74 | |
| PMF | | 0.29 | 0.21 | 0.19 | | | | | 0.1 | | | 0.13 | | | | 89.0 | | 0.17 | | | | 0.39 | | | | 66.0 | | _ | | _ | | | | | | | |
| Verify score | | 0.21 | 20:0 | 0 | | | | 1 | 90.0- | | | -0.25 | | | | 80.0 | | 0.17 | | | | 0.41 | | | | 0.41 | | 89.0 | | 0.12 | | | | | | | |
| PSI- BLAST | | 5.40E-26 | 5.40E-31 | 5.40E-33 | | | | | 1.30E-29 | | | 3.60E-26 | | | | 3.60E-21 | | 9.00E-26 | | | | 9.00E-28 | | | | 1.30E-24 | | 6.50E-24 | 7000. | 1.10E-34 | | | | | | 5.40E-39 | |
| End | | 297 | 297 | 297 | | | | | 337 | | | 337 | | _ | | 274 | | 297 | | | | 297 | | | | 228 | | 161 | 0.0 | 739 | | | | | | 230 | |
| Start AA | | 142 | 142 | 142 | | | | | 131 | | | 139 | | | | 135 | | 142 | | | | 142 | | | | 112 | | * | 5 | 711 | | | | | | 73 | |
| Chain ID | | ٧ | ٧ | O | | | | | 4 | | | В | | | | ¥ | | 4 | | | | ٧ | | | | | | | 6 | n | | | | | | В | |
| PDB | | 1694 | 169ľ | 1613 | | | | | 3 | 6 | | lcla | | | | lcxq | | lexd | | | 1 | 1 ds4 | | | - | laSe | 1 | lase | Torres | Iawc | | | | | | lawc | |
| SEQ No de | | 715 | 715 | 715 | | | | , | 715 | | | 715 | | | | 715 | | 715 | | | 1 | 715 | | | | 419 | | 5 | 910 | - | | | | | | 719 | |

| PDB annotation | REGULATIONIONA) GABPALPHA; GABBERTA; COMPLEX (TRANSCRIPTION REGULATIONIONA), DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR. | COMPLEX (TRANSCRIPTION REGULATIONINA) ADBRALPHI, GABPBETAL; COMPLEX (TRANSCRIPTION REGULATIONINA), DIM-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKTRIN REPEATS, TRANSCRIPTION 3 FACTOR. | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | COMPLEX (KINASZBANTI- ONCOGENB) CDKG, PIGNK4A, MTS1; CYCLIN DEPENDENT KINASE CYCLIN DEPENDENT KINASE FHHISTORY 2 PROTEIN, CDK, INK4, CELL CYCLE, MULTILE TUMOR SUPPRESSOR, 3 MTS1, COMPLEX KINASZBANTI-ONCOGENBI HEADER | COMPLEX (INHIBITOR PROTEINMANASI) NHBITOR PROTEIN, CYCLIN-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHANEET, COMPLEX (INHIBITOR PROTEINKINASE) |
|------------------|---|--|--|--|--|--|---|---|
| Coumpound | ALPHA; CHAIN: A; GA BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN ALPHA; CRANY: A; GA BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; | P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | PI9INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | CYCLIN-DEPENDENT KIANSE G, CHARIN A; MULTIPLE TUMOR SUPPRESSOR; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B; |
| SeqFold score | | | | 68.17 | | | | |
| PMF score | | _ | 0.51 | | | - | - | 0.36 |
| Verify score | | 0.32 | 90.0 | | 0.77 | 0.13 | 0.33 | 0.21 |
| PSI- BLAST | | 5.40E-39 | 1.10E-25 | 7.80E-35 | 7.80E-35 | 1.10E-34 | 1.40E-25 | 9.00E-24 |
| End | | 228 | 091 | 233 | 218 | 231 | 228 | 160 |
| Start AA | | 78 | 21 | 73 | 78 | 78 | 112 | 21 |
| Chain 10 | | g . | | | | | m. | щ |
| PDB ID | | Івис | 1bd8 | 1bd8 | 8pq1 | 1bd8 | 7141 | 1bk |
| SEQ No. | | 719 | 617 | 719 | 719 | 612 | 719 | 719 |

| PDB annotation | COMPLEX (INHIBITOR PROTEIN, CAMPLEX (INHIBITOR PROTEIN, CYCLIA-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHABETA, COMPLEX (INHIBITOR PROTEINKINASE). | COMPLEX (INHIBITOR PROTEINKINASE) INHIBITOR PROTEIN, CYCLIA-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHANEET, COMPLEX (INHIBITOR PROTEINKINASE) | COMPLEX (INHIBITOR PROTEIN/CHASE) NHIBITOR PROTEIN, CYCLIA-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHANEET, COMPLEX (INHIBITOR PROTEIN/KINASE) | HORMONE/GRO WTH FACTOR P18- INK4C; CELL CYCLE INHBITOR, P18INK4C; TUMOR, SUPPRESSOR. CYCLIN-2 DEPENDENT KINASE, HORMONE/GROWTH FACTOR | HORMONE/GROWTH FACTOR P18- INKAC, CELL CYCLE INHBITOR, P18INKAC, TUMOR, SUPRESSOR, CYCLIN-2 DEPENDENT KINASE, HORMONE/GROWTH FACTOR | HORMONE/GROWTH FACTOR P18- INK4C; CELL CYCLE INHBITOR, P18INK4C; TUMOR, SUPRESSOR, CYCLIN-2 DEPENDENT KINASE, HORMONE/GROWTH FACTOR. | SIGNALING PROTEIN HELIX-TURN- HELIX, ANKYRIN REPEAT | SIGNALING PROTEIN HELIX-TURN- HELIX, ANKYRIN REPEAT | SIGNALING PROTEIN HELIX-TURN- HELIX, ANKYRIN REPEAT |
|------------------|--|---|---|---|---|--|--|--|--|
| Coumpound | CYCLIN-DEPENDENT KINASE 6, CHAIN: A; PI 9INKAD; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INKAD; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A; | CYCLIN-DEPENDENT KINASE 4 INHIBITOR B; CHAIN: A; | CYCLIN-DEPENDENT KINASE 4 INHIBITOR B; CHAIN: A; | CYCLIN-DEPENDENT KINASE 4 INHIBITOR B; |
| SeqFold score | 70.26 | | | | 67.41 | | | | |
| PMF | | - | _ | 0.12 | | - . | _ | 66:0 | - |
| Verify | | 0.62 | 0.39 | -0.07 | | 0.17 | 0.33 | 0.48 | 0.73 |
| PSI- BLAST | 1.30E-35 | 1.30E-35 | 3.60E-34 | 1.10E-25 | 1.10E-36 | 1.10E-36 | 2.60E-29 | 1.10E-25 | 1.20E-28 |
| End | 201 | 218 | 231 | 591 | 239 | 233 | 218 | 234 | 197 |
| Start | 4 | | 78 | 81 | 0, | 78 | 101 | 112 | 78 |
| Chain | æ | м | ш | ∢ | < | ⋖ | ¥. | < | < |
| PDB CI | 191 Xq1 | 1blx | 1blx | lbu9 | 1bu9 | Ibu9 | 149s | 1498 | s6p1 |
| SE O | 719 | 917 | 719 | 719 | 719 | 917 | 719 | 719 | 917 |

| PDB annotation | | CELL CYCLE INHIBITOR P18. INK4C(INK6); CELL CYCLE INHIBITOR, P18-INK4C(INK6), ANK YRIN REPEAT, 2 CDK 4/6 INHIBITOR. | CELL CYCLE INHIBITOR PIB- INK4C(INK6); CELL CYCLE INHIBITOR, PIB-INK4C(INK6), ANKYRIN REPEAT, 2 CDK 4/6 INHIBITOR. | CELL CYCLE INHIBITOR P18- NR4C(INK6); CELL CYCLE INHIBITOR, P18-NR4C(INK6), ANKYRIN REPEAT, 2 CDK 4/6 INHIBITOR. | CELL CYCLE INHIBITOR P18- INK4C(INK6); CELL CYCLE INHIBITOR, P18-INK4C(INK6), ANKYRIN REPEAT, 2 CDK 4/6 INHIBITOR | TRANSCRIPTION FACTOR, P65; P50D; TRANSCRIPTION FACTOR, IKBAFKB COMPLEX | TRANSCRIPTION FACTOR P65; P30D; TRANSCRIPTION FACTOR, IKBANFKB COMPLEX | TRANSCRIPTION FACTOR, P63; P50D; TRANSCRIPTION FACTOR, IKBANFKB COMPLEX | TRANSCRIPTION FACTOR P65; P30D; TRANSCRIPTION FACTOR, IKBNFKB COMPLEX | TRANSCRIPTION FACTOR P65; P30D; TRANSCRIPTION FACTOR, IKBNFKB COMPLEX |
|------------------|-----------|---|--|--|---|---|---|--|---|---|
| Coumpound | CHAIN: A; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA; CHAIN: D; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA; CHAIN: D; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-AI PHA: CHAIN: D: | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT: CHAIN: C; I- KAPPA-B-ALPHA: CHAIN: D: | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA; CHAIN: D; |
| SeqFold score | | | | 63.76 | | | | 69.17 | | |
| PMF | | 90.0 | 0.93 | | 1 | 0.33 | 6.0 | | 69:0 | 0.76 |
| Verify score | L | -0.2 | 0.31 | | 0.24 | -0.33 | -0.04 | | -0.05 | -0.21 |
| PSI- BLAST | | 1.40E-21 | 5.40E-25 | 5.40E-36 | 5.40E-36 | 3.60E-26 | 3.60E-33 | 7.20E-39 | 7.20E-39 | 1.30E-27 |
| End | | 131 | 164 | 232 | 232 | 238 | 171 | 216 | 228 | 144 |
| Start | | - | 81 | 75 | 78 | 107 | 13 | 21 | 39 | s |
| Chain ID | | ٧ | < | < | ∢ | Q | Q | Ω | Ω | Ω |
| PDB CI | | lihb | <u>a</u> | | 1ihb | lik | likn | 털 | lika | likn |
| S e S | | 719 | 719 | 719 | 719 | 719 | 917 | 719 | 719 | 719 |

| | | | | | | | | | | | | | | | | | | | | | | | _ | | | | | | | | |
|-----------------|--|--|---------------------------|--|---------------------------------|---------------------------|---------------------------|--|---------------------------|---------------------------|--|---------------------------|---------------------------|-------------------------------|----------------------------------|-----------------------|----------------------------|-------------------------------|--------------------------|--------------------------|---------------------------|---------------------------|---|------------------------|-------------------------|-----------------------------|---------------------------------|------------------------------|--|------------------------|-------------------------|
| PDB annotation | ANK-REPEAT MYOTROPHIN, ACETYLATION, NMR, ANK-REPEAT | ANK-REPEAT MYOTROPHIN, ACETYLATION, NMR, ANK-REPEAT | COMPLEX (TRANSCRIPTION | REGIANK REPEAT) COMPLEX (TRANSCRIPTION REGIT, ATTON/ANK | REPEAT), ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION | REG/ANK REPEAT) COMPLEX | (TRANSCRIPTION REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION | REG/ANK REPEAT) COMPLEX | (TRANSCRIPTION REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION | REG/ANK REPEAT) COMPLEX | (TRANSCRIPTION REGULATION/ANK | KEPEAL), ANK YKIN 2 KEPEAL HELIX | COMPLEX (ANII- | UNCOGENE/AIN TRIN REFEATS) | TUMOR SUPPRESSOR, MULTIGENE 2 | FAMILY, NUCLEAR PROTEIN, | PHOSPHORYLATION, DISEASE | MUTATION, 3 POLYMORPHISM, | ONCOGENE/ANKYRIN REPEATS) | | COMPLEX (TRANSCRIPTION | GABPBETA I: COMPLEX | (TRANSCRIPTION | REGULATION/DNA), DNA-BINDING, 2 | NUCLEAR PROTEIN, ETS DOMAIN, | ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR | COMPLEX (TRANSCRIPTION | GABPBETA1; COMPLEX |
| Coumpound | MYOTROPHIN; CHAIN: NULL | MYOTROPHIN; CHAIN: NULL | NF-KAPPA-B P65; CHAIN: A, | C; NF-KAPPA-B P50; CHAIN: B D: L.K APPA-R-AI PHA: | CHAIN: E, F; | NF-KAPPA-B P65; CHAIN: A, | C, NF-KAPPA-B P50, CHAIN: | B, D; I-KAPPA-B-ALPHA; CHAIN: E, F; | NF-KAPPA-B P65; CHAIN: A, | C; NF-KAPPA-B P50; CHAIN: | B, D; I-KAPPA-B-ALPHA; | NF-KAPPA-B P65; CHAIN: A, | C; NF-KAPPA-B P50; CHAIN: | B, D; I-KAPPA-B-ALPHA; | CHAIN: E, F; | P53; CHAIN: A; 53BP2; | CHAIN: B; | | | | | | | GA BINDING PROTEIN | BINDING PROTEIN BETA 1: | CHAIN: B; DNA; CHAIN: D, E; | | | | GA BINDING PROTEIN | BINDING PROTEIN BETA 1; |
| SeqFold | | 64.15 | | | | | | | | | | 99:59 | | | | 64.29 | | | | | | | | | | | | | | | |
| PMF | 1 | | 0.94 | | | 0.92 | | | 0.78 | | | | | | | | | | | | | | | 1 | | | | | | _ | |
| Verify score | 0.14 | | 0.19 | | | -0.07 | | | 0.07 | | | | | | | | | | | | | | | 0.79 | | | | | | 0.83 | |
| PSI- BLAST | 2.60E-28 | 6.50E-33 | 9.00E-26 | | | 9.00E-33 | | | 1.10E-38 | | | 1.10E-38 | | | | 1.60E-20 | | | | | | | | 7.80E-42 | | | | | | 2.60E-42 | |
| End | 225 | 192 | 238 | | | 111 | | | 228 | | | 202 | | | | 239 | | | | | | | | 312 | | | | | | 147 | |
| Start | 110 | 75 | 106 | | | 12 | | | 39 | | | 7 | | | | 74 | | | | | | | | 191 | | | | | | 2. | |
| Chain | | | E | | | Ξ | | | E | | | Е | | | | 20 | | | | | | | | В | | | | | | В | |
| 80 a | lmy o | Jil o | 91 | | | inf. | | | Iufi | | | Infi | | | | lyes | | | | | | | I | lawc | | | | | | lawc | |
| S e S | 719 | 719 | 119 | | | 719 | | | 119 | | | 719 | | | | 719 | | | | | | | | 721 | | | | | | 721 | |

| PDB annotation | (TRANSCRIPTION REGULATIONDNA), DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR. | COMPLEX (TRANSCRIPTION REGULATIONDNA) CABRALPHA; GABPERTAI; COMPLEX (TRANSCRIPTION REGULATIONDNA), DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN ANKYRIN REPEATS, TRANSCRIPTION ANKYRIN REPEATS, TRANSCRIPTION | COMPLEX (TRANSCRIPTION REQUILT/DIONNYA GBRALPHA; GABPETA; COMPLEX (TRANSCRIPTION REGULATION/DNA, DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN ANKYRIN REPEATS, TRANSCRIPTION 3 PACTOR | COMPLEX (TRANSCRIPTION REGULATIONONA) COBPALPHA; GABPERTA; COMPLEX (TRANSCRIPTION REGULATIONIONA), DNA-BINDING; 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS; TRANSCRIPTION 3 PACTOR | COMPLEX (TRANSCRIPTION REGULATIONONA) CABBALPHA; GABBETA I; COMPLEX (TRANSCRIPTION REGULATIONIDAA) DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS; TRANSCRIPTION | COMPLEX (TRANSCRIPTION REGULATION/DNA) GABPALPHA; GABPBETA1; COMPLEX (TRANSCRIPTION |
|----------------|---|---|---|--|---|---|
| Coumpound | CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN ALPHA; CHANI: A; GA BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN HETHA; CHAIN: A; GA BINDING PROTEIN BETA I; CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN ALPHA; CHAIN: A; GA BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN HAHA, CERNIC A; GA BINDING PROTEIN BETA I; CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN ALPHA; CHAIN: A: GA BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; |
| SeqFold | | | | | | |
| PMF | | - | _ | _ | _ | - |
| Verify | | 0.71 | 4. | 0.72 | 0.9 | 1.23 |
| PSI- BLAST | | 3.60E-34 | 5.20E-43 | 1.30E-44 | 3.60E-39 | 5.20E-45 |
| End | | 147 | 378 | 180 | 378 | 412 |
| Start AA | | 7 | 226 | 23 | 231 | 259 |
| Chain ID | | Д | ш | Ø | m | æ |
| PDB DD | | lawc | lawc | lawc | lawc | lawc |
| SEQ NO: | | 721 | 721 | 721 | 121 | 721 |

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|-----------------|---|---|--|--|---|--|
| PDB annotation | REGULATION/DNA), DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR | COMPLEX (TRANSCRIPTON REGULATIONIDAN, OBBPALPHA; GABPBETAI; COMPLEX (TRANSCRIPTON REGULATIONIDA), DIA-BINDING, 2 REGULATIONIDA, DIA-BINDING, 2 NUCLEAR PROTEIN, FIYS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR. | COMPLEX (TRANSCRIPTION REGIL-ATIONDNA), OBBALPHA; GARPBETA; COMPLEX (TRANSCRIPTION REGIL-ATIONDNA), DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAN, ANKYRIN REPEATS, TRANSCRIPTION S PACTOR. | COMPLEX (TRANSCRIPTION REGULATIONDNA) ADBRALPHA; . GABBETA; COMPLEX (TRANSCRIPTION REGULATION/DA), DAV. BINDING, 2 NUCLEAR PROTEIN, ETS DOMAN, ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR. | COMPLEX (TRANSCRIPTION REGILATIONDN/A DOBPALPHA; GABBETA; COMPLEX (TRANSCRIPTION REGILATION/DA, DNA.BNDING, 2 NUCLEAR PROTEIN, ETS DOMAN, ANKTRIN REPEATS, TRANSCRIPTION 3 FACTOR. | COMPLEX (TRANSCRIPTION REGULATIONDNA) GABPALPHA; COMPLEX (TRANSCRIPTION REGULATIONDNA), DNA-BINDING, 2 |
| Coumpound | | GA BINDING PROTEIN ALPHA, CRAIN: A; GA BINDING PROTEIN BETA 1; CHAIN: B; DIA; CHAIN: D, E; | GA BINDING PROTEIN LEHA, CHARIN, A; GA BINDING PROTEIN BETA I; CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN ALPHA; CHAIN: A: GA BINDING PROTEIN BETA 1; CHAIN: B: DNA; CHAIN: D, E; | GA BINDING PROTEIN ALPHA; CRAIN: A; GA BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN ALPHA; CHAIN: A; GA BINDING PROTEIN BETA I; CHAIN: B; DNA; CHAIN: D, E; |
| SeqFold | | | | | | |
| PMF | | _ | _ | _ | _ | 0.62 |
| Verify score | | 0.93 | 0.93 | 0.69 | 0.67 | 0.22 |
| PSI- BLAST | | 5.40E-41 | 1.80E-36 | L.30E-38 | 1.80E-36 | 7.20E-32 |
| End | | 411 | 442 | 180 | 475 | 487 |
| Start | | 264 | 297 | 33 | 330 | 363 |
| Chain ID | | я | æ | æ | В | В |
| 908 E1 | | lawc | Тамс | lawc | Тамс | lawc |
| SE SE | | 121 | 721 | 721 | 721 | 721 |

| PDB annotation | NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR | COMPLEX (TRANSCRETTON REGULATIONDNA) OBBALPHA; GABPETAI; COMPLEX (TRANSCRETTON REGULATIONDNA), DNA-BINDDNG, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKTRIN REPEATS, TRANSCRETTON | COMPLEX (TRANSCRIPTION REGULATIONINA), OBPALPHA; GABBETAI; COMPLEX (TRANSCRIPTION REGULATIONINA), DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION 3 PACTOR. | COMPLEX (TRANSCRIPTION REGULATIONDNA) GABPALPHA; GABBETAI; COMPLEX (TRANSCRIPTION REGULATIONONA), DNA-BINDDNG, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKTRIN REPEATS, TRANSCRIPTION 3 PACTOR. | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, |
|-----------------|--|--|---|---|--|--|--|--|---|
| Coumpound | | GA BINDING PROTEIN ALPHA; CHANI: A; GA BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN ALPHA; CHAINLA; GA BINDING PROTEIN BETA I; CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN ALPHA: CHAIN: A; GA BINDING PROTEIN BETA I; CHAIN: B; DNA; CHAIN: D, E; | P19TNK4D CDK4/6 DNHIBITOR; CHAIN: NULL; | P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL; |
| SeqFold | | | | | | | | | |
| PMF score | | - | _ | - | _ | 0.42 | 1 | 1 | 1 |
| Verify score | | 0.59 | 0.79 | 0.87 | 0.79 | 0.12 | 0.43 | 0.73 | 0.53 |
| PSI- BLAST | | 6.50E-47 | 1.40E-39 | 5.40E-38 | 2.60E-38 | 2.60E-38 | 1.20E-40 | 9.10E-41 | 1.30E-41 |
| End | | 213 | 213 | 246 | 281 | 348 | 149 | 381 | 182 |
| Start AA | | 61 | 99 | 66 | 128 | 161 | | 227 | 24 |
| Chain ID | | æ | æ | В | | | | | |
| PDB CI | | lawc | lawc | lawc | 15d8 | 1bd8 | 1bd8 | 1bd8 | 1Pd8 |
| SEQ B B S | | 721 | 721 | 721 | 121 | 121 | 721 | 721 | 721 |

| | _ | | | _ | | | | | | _ | | | _ | | _ | | _ | _ | | _ | | _ | _ | | _ | _ | | _ | _ | | _ |
|--|---------------|--|---|----------------|--|--------------------|--------------------------|-------------------------------|--|--------------------|---------------------------|---------------------------|-------------------------------|--|--------------------|---------------------------|---------------------------|-------------------------------|--|--------------------|---------------------------|---------------------------|-------------------------------|--------------------------------|-----------------|--------------------|---------------------------|---------------------------|-------------------------------|--|--------------------|
| PDB annotation | ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, | ANK YRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | COMPLEX (INHIBITOR | PROTEIN CYCLIN-DEPENDENT | KINASE, CELL CYCLE 2 CONTROL, | ALPHA/BETA, COMPLEX (INHIBITOR PROTEIN/KINASE) | COMPLEX (INHIBITOR | PROTEIN/KINASE) INHIBITOR | PROTEIN, CYCLIN-DEPENDENT | KINASE, CELL CYCLE 2 CONTROL, | ALPHA/BETA, COMPLEX (INHIBITOR PROTEIN/KINASE) | COMPLEX (INHIBITOR | PROTEIN/KINASE) INHIBITOR | PROTEIN, CYCLIN-DEPENDENT | KINASE, CELL CYCLE 2 CONTROL, | ALPHA/BETA, COMPLEX (INHIBITOR PROTEIN/KINASE) | COMPLEX (INHIBITOR | PROTEIN/KINASE) INHIBITOR | PROTEIN, CYCLIN-DEPENDENT | KINASE, CELL CYCLE 2 CONTROL, | ALPHA/BETA, COMPLEX (INHIBITOR | PROTEIN/KINASE) | COMPLEX (INHIBITOR | PROTEIN/KINASE) INHIBITOR | PROTEIN, CYCLIN-DEPENDENT | KINASE, CELL CYCLE 2 CONTROL, | ALFHA/BETA, COMPLEX (INHIBITOR PROTEIN/KINASE) | COMPLEX (INHIBITOR |
| Coumpound | | PI9INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | | P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | CYCLIN-DEPENDENT | NINASE 6; CHAIN: A; | | | CYCLIN-DEPENDENT | KINASE 6; CHAIN: A; | P19INK4D; CHAIN: B; | | | CYCLIN-DEPENDENT | KINASE 6; CHAIN: A; | P19INK4D; CHAIN: B; | | | CYCLIN-DEPENDENT | KINASE 6; CHAIN: A; | P19INK4D; CHAIN: B; | | | | CYCLIN-DEPENDENT | KINASE 6; CHAIN: A; | PI9INK4D; CHAIN: B; | | | CYCLIN-DEPENDENT |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 1 | _ | | _ | _ | | | | _ | | | | | | | | | | | | | | | | _ | | | | | _ |
| Verify score | | 68'0 | 0.74 | | 0.67 | 0.83 | | | | 0.13 | | | | | 0.81 | | | | | 19.0 | | | | | | 0.78 | | | | | 1.13 |
| PSI- BLAST | | 1.20E-38 | 1.40E-30 | | 7.80E-44 | 1.30E-39 | | | | 5.20E-38 | | | | | 1.00E-41 | | | | | 6.50E-43 | | | | | | 1.30E-43 | | | | | 5.20E-41 |
| End | | 414 | 442 | | 215 | 282 | | | | 350 | | | | | 153 | | | | | 185 | | | | | 1 | ž Ž | | | | | 416 |
| Start AA | | 263 | 297 | | 62 | 132 | | | | 163 | | | | | 2 | | | | | 22 | | | | | | 062 | | | | | 263 |
| Chain ID | | | | | | В | | | | m | | | | | В | | | | | В | | | | | | 1 0 | | | | | В |
| PDB CD | | 8pq1 | 15d8 | | 15d8 | 1blx | | | | 1blx | | | | | 1bk | | | | | 1bk | | | | | 1 | × | | | | | 1blx |
| SE Si Si Si Si Si Si Si Si Si Si Si Si Si | | 121 | 121 | 7 | 121 | 721 | | | | 721 | | | | | 721 | | | | | 721 | | | | | į | 17/ | | | | | 721 |

| PDB annotation | PROTEIN/KINASE) INHIBITOR PROTEIN, CYCLIN-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHA/BETA, COMPLEX (INHIBITOR PROTEIN/KINASE) | COMPLEX (INHIBITOR PROTEINING ASSISTANCE) PROTEINING ASSISTANCE AS | HORMONE/GROWTH FACTOR P18- INK4C; CELL CYCLE INHBITOR, P18INK4C; TUMOR, SUPPRESSOR, CYCLIN-2 DEPENDENT KINASE, HORMONE/GROWTH FACTOR | HORMONE/GROWTH FACTOR P18- INKAC; CELL CYCLE INHBITOR, P18INKAC; TUMOR, SUPPRESSOR, CYCLIN-2 DEPENDENT KINASE, HORMONE/GROWTH FACTOR | HORMONE/GRO WTH FACTOR P18- INKAC, CELL CYCLE INHIBITOR, P1 BINKAC, TUMOR, SUBPRESSOR, CYCLIN- 2 DEPENDENT KINASE, HORMONE/GROWTH FACTOR | SIGNALING PROTEIN HELIX-TURN- HELIX, ANKYRIN REPEAT | SIGNALING PROTEIN HELIX-TURN- HELIX, ANKYRIN REPEAT | SIGNALING PROTEIN HELIX-TURN- HELIX, ANKYRIN REPEAT | SIGNALING PROTEIN HELIX-TURN- HELIX, ANKYRIN REPEAT | SIGNALING PROTEIN HELIX-TURN- HELIX, ANKYRIN REPEAT |
|------------------|--|--|--|--|--|--|--|--|--|--|
| Coumpound | KINASE 6; CHAIN: A; PI9INK4D; CHAIN: B; | . CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A; | CYCLIN-DEPENDENT KINASE 4 INHIBITOR B; CHAIN: A; | CYCLIN-DEPENDENT KINASE 4 INHIBITOR B; CHAIN: A; | CYCLIN-DEPENDENT KINASE 4 INHIBITOR B; CHAIN: A: | CYCLIN-DEPENDENT KINASE 4 INHIBITOR B; CHAIN: A; | CYCLIN-DEPENDENT KINASE 4 INHIBITOR B; CHAIN: A; |
| SeqFold score | | | | | 90.26 | | | | | |
| PMF | | - | - | 0.35 | | - | - | _ | _ | 1. |
| Verify score | | 0.39 | 0.61 | 0.37 | | 9.0 | 0.66 | 0.58 | 0.65 | 0.61 |
| PSI- BLAST | | 6.50E-43 | 7.20E-38 | 1.80E-32 | 7.20E-38 | 6.50E-36 | 1.30E-37 | 1.30E-40 | 2.60E-38 | 2.60E-38 |
| End AA | | 252 | 185 | 480 | 258 | 153 | 384 | 416 | 185 | 216 |
| Start AA | | 49 | 33 | 330 | 16 | 14 | 250 | 283 | 52 | 84 |
| Chain TD | | e e | ∢ | ∢ | v | ٧ | Ą | A | ٧ | < − |
| EDB CD | | 1blx | 1bu9 | 1bu9 | 1bu9 | 1498 | 1d9s | s6PI | 149s | 1498 |
| SEQ NO: | | 121 | 721 | 721 | 121 | 721 | 721 | 721 | 721 | 721 |

| PDB annotation | CELL CYCLE INHIBITOR P18- INK4CINK6); CELL CYCLE INHIBITOR, P18-INK4CINK6), ANYYRIN REPEAT, 2 CDK 4/6 INHIBITOR. | CELL CYCLE INHIBITOR P18- INK4C(INK6); CELL CYCLE INHIBITOR, P18-INK4C(INK6), ANYNIN REPEAT, 2 CDK 4/6 INHIBITOR. | CELL CYCLE NHIBITOR P18- NK4C(NK6); CELL CYCLE NHIBITOR, P18-NK4C(NK6), AHYYRIN REPEAT, 2 CDK 4/6 NHIBITOR | CELL CYCLE INHIBITOR P18- INK4C(INK6); CELL CYCLE INHIBITOR, P18-INK4C(INK6), ANYYRIN REPEAT, 2 CDK 4/6 INHIBITOR. | TRANSCRIPTION FACTOR P65, P50D; TRANSCRIPTION FACTOR, IKBNFKB COMPLEX | TRANSCRIPTION FACTOR P65; P50D; TRANSCRIPTION FACTOR, IKBNFKB COMPLEX | TRANSCRIPTION FACTOR P65, P50D; TRANSCRIPTION FACTOR, IKBNFKB COMPLEX | TRANSCRIPTION FACTOR P65; P50D; TRANSCRIPTION FACTOR, IKBNFKB COMPLEX | TRANSCRIPTION FACTOR P65, P50D; TRANSCRIPTION FACTOR, IKBNFKB COMPLEX | TRANSCRIPTION FACTOR P65; P50D; |
|------------------|--|---|--|--|---|---|---|--|--|---------------------------------|
| Coumpound | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; 1- KAPPA-B-ALPHA; CHAIN: D; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA; CHAIN; D; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA; CHAIN: D; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; 1- KAPPA-B-AI,PHA: CHAIN: D: | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-AI PHA: CHAIN: D: | NF-KAPPA-B P65 SUBUNIT; |
| SeqFold score | | | | 88.22 | 82.11 | | | | | |
| PMF | _ | _ | 0.92 | | | 0.93 | 66.0 | _ | - | 0.39 |
| Verify score | 0.7 | 0.55 | 0.5 | | | -0.02 | 0.48 | 0.56 | 0.55 | 0.4 |
| PSI- BLAST | 1.80E-32 | 3.60E-37 | 1.305-31 | 3.60E-37 | 2.60E-57 | 2.60E-55 | 5.20E-52 | 5.40E-43 | 7.80E-52 | 7.20E-39 |
| End | 446 | 184 | 479 | 250 | 333 | 386 | 188 | 411 | 416 | 475 |
| Start AA | 297 | 33 | 330 | 96 | 127 | 191 | 2 | 226 | 226 | 292 |
| Chain ID | ٧ | ¥ | ¥ | ٧ | D | D | D | Q | Q | D |
| PDB DD | 11116 | lib | lihb | lihb | lika | 1ikn | М | likn | lik I | liku |
| SEQ NO: | 721 | 721 | 721 | 721 | 121 | 721 | | 721 | 121 | 721 |

| PDB annotation | TRANSCRIPTION FACTOR, IKBNFKB COMPLEX | TRANSCRIPTION FACTOR, P65; P30D; TRANSCRIPTION FACTOR, IKBNFKB COMPLEX | TRANSCRIPTION FACTOR P63; P30D; TRANSCRIPTION FACTOR, IKB/NFKB COMPLEX | TRANSCRIPTION FACTOR P65; P30D; TRANSCRIPTION FACTOR, IKB/NFKB COMPLEX | COMPLEX (TRANSCRIPTION REG/ANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION REGANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT) ANKYRN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION REGANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT) ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION REGIANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT) ANKYRN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION REGIANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT) ANKYRN 2 REPEAT HEILY | COMPLEX (TRANSCRIPTION RECIANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT) ANKYRN 2 REPEAT HEINX | COMPLEX (TRANSCRIPTION REG/ANK REPEAT) COMPLEX |
|------------------|--|---|---|---|--|---|--|--|--|---|--|
| Coumpound | CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; J- KAPPA-B-ALPHA; CHAIN: D; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NP-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA: CHAIN: D: | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA: CHAIN: D; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA; CHAIN: D; | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E, F; | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E. F: | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E, F; | NF.KAPPA-B P65; CHAIN: A, C; NF.KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E, F. | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E. F. | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B. D; I-KAPPA-B-ALPHA; CHAIN: E. F: | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: |
| SeqFold score | | | | | 85.42 | | | | | | |
| PMF | | 0.05 | _ | _ | | - | - | _ | _ | _ | _ |
| Verify score | | 60:0 | 0.2 | 0.22 | | 0.08 | 69:0 | 0.49 | 0.82 | 8.0 | 0.65 |
| PSI- BLAST | | 7.20E-34 | 5.40E-38 | 2.60E-57 | 2.60E-52 | 2.60E-52 | 7.80E-42 | 7.80E-53 | 7.20E-43 | 6.50E-52 | 1.60E-38 |
| End | | 486 | 233 | 256 | 322 | 350 | 153 | 216 | 411 | 420 | 475 |
| Start AA | | 325 | 19 | 19 | 124 | 124 | 2 | 21 | 224 | 226 | 292 |
| Chain D | | Q | Δ | Ω | ш | ш | ы | 1 | щ | മ | Е |
| PDB ID | | Jik M | rii Fi | ljki m | Infi | ĮĮ. | lnfi | Jug | Înî | Juf | Infi |
| SEQ D NO: | | 121 | 121 | 721 | 721 | 721 | 721 | 721 | 121 | 121 | 121 |

| PDB annotation | (TRANSCRIPTION REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION REG/ANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK | REPEAT), ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION REGULATION/DNA) GABPALPHA; GABPBETA; COMPLEX | (TRANSCRIPTION REGULATIONIDNA), DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION | COMPLEX (TRANSCRIPTION | REGULATION/DNA) GABPALPHA; | (TRANSCRIPTION | REGULATION/DNA), DNA-BINDING, 2 | ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR | COMPLEX (TRANSCRIPTION | KEGULATION/DNA) GABPALPHA; GABPBETA1; COMPLEX | (TRANSCRIPTION | REGULATION/DNA), DNA-BINDING, 2 | ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR | COMPLEX (TRANSCRIPTION | REGULATION/DNA) GABPALPHA; | GABPBETAI; COMPLEX CTRANSCRIPTION | REGULATION/DNA), DNA-BINDING, 2 | NUCLEAR PROTEIN, ETS DOMAIN, | ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR | COMPLEX (TRANSCRIPTION REGULATION/DNA) GABPALPHA; |
|------------------|--|--|---------------------------------|---|--|------------------------|----------------------------|-----------------------------|---------------------------------|--|------------------------|--|-----------------------------|---------------------------------|---|------------------------|----------------------------|--------------------------------------|---------------------------------|------------------------------|--|---|
| Coumpound | B, D; I-KAPPA-B-ALPHA; CHAIN: E, F; | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; | CHAIN: E, F; | GA BINDING PROTEIN ALPHA, CHAIN: A; GA BINDING PROTEIN BETA 1; | CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN | ALPHA: CHAIN: A; GA | CHAIN: B; DNA; CHAIN: D, E; | | | GA BINDING PROTEIN | ALPHA; CHAIN: A; GA BINDING PROTEIN BETA 1; | CHAIN: B; DNA; CHAIN: D, E; | | | GA BINDING PROTEIN | ALPHA; CHAIN: A; GA | CHAIN B. DNA: CHAIN: D. P. | | | | GA BINDING PROTEIN ALPHA; CHAIN: A; GA |
| SeqFold score | | | | | | | | | | | | | | | | 64.41 | | | | | | |
| PMF | | 96.0 | | - | | 0.64 | | | | | -0.17 | | | | | | | | | | | 1 |
| Verify score | | 0.52 | | 0.32 | | 0.4 | | | | | 0.02 | | | | | | | | | | | 0.35 |
| PSI- BLAST | | 1.80E-33 | | 1.60E-31 | | 1.60E-23 | | | | | 3.60E-30 | | | | | 5.40E-36 | | | | | | 5.40E-36 |
| End AA | | 486 | | 280 | | 343 | | | | | 408 | | | | | 198 | | | | | | 157 |
| Start AA | | 323 | | 107 | | 175 | | | | | 265 | | | | | 31 | | | | | | 9 |
| Chain ID | | Э | | В | | В | | | | | В | | | _ | | В | | | | | | В |
| PDB TD | | infi | | lawc . | | lawc | | | | | lawc | | | | | lawc | | | | | | lawc |
| SEQ NO: | | 121 | | 723 | | 723 | | | | | 723 | | | | | 723 | | | | | | 723 |

| PDB annotation | GABPBETA1; COMPLEX (TRANSCRIPTION REGULATION/DNA, DNA-BINDING, 2 NUCLEAR REOTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR | COMPLEX (TRANSCRIPTION REGULATION/DNA (DBPALPHA; GABBERTA; COMPLEX (TRANSCRIPTION 2 REGULATION/DNA, DNA-BINDING, 2 NUCLEAR PROTTEN, ETS DOMAN, ANKYRIN REPEATS, TRANSCRIPTION 3 PACTOR | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF | COMPLEX (INHIBITOR PROTEINCAS) PROTEINCHASE) INHIBITOR PROTEINCHASE) CHALLOEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHANEST, COMPLEX (INHIBITOR PROTEINKINASE) | COMPLEX (INHIBITOR PROTEINICHASE) HHBITOR PROTEINICACION-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHAMETA, COMPLEX (INHIBITOR PROTEINICHASE) | HORMONEGROWTH FACTOR P18- INKAC, CELL CYCLE INHIBITOR, P18INKAC, TUMOR, SUPPRESSOR, CYCLIN- 2 DEPENDENT KINASE, HORMONEGROWTH FACTOR | HORMONE/GROWTH FACTOR P18- |
|------------------|--|--|--|--|--|--|---|--|----------------------------|
| Coumpound | BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; | GA BINDING PROTEIN ALPHA, CHAIN: A; CA BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; | PI9INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | PI9INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A; | CYCLIN-DEPENDENT |
| SeqFold score | | | 56.93 | | - | | | | |
| PMF | | _ | | - | - | - | - | 0.3 | 96:0 |
| Verify score | | 0.71 | | 0.43 | 0.21 | 0.44 | 0.44 | 0.24 | 0.25 |
| PSI- BLAST | | 2.60E-27 | 3.60E-29 | 7.20E-27 | 3.60E-29 | 2.60E-26 | 5.40E-29 | 3.60E-29 | 5.40E-34 |
| End AA | | 212 | 201 | 182 | 160 | 202 | 148 | 291 | 162 |
| Start | | 72 | 38 | 43 | 6 | 43 | 6 | 107 | 9 |
| Chain ID | | g | | | | B | Ω | ∢ | Ą |
| PDB OU | | lawc | 1bd8 | 1bd8 | 3pqI | 1blx | 1bk | 1bu9 | 1bu9 |
| SEQ NO ID | | 723 | 723 | 723 | 723 | 723 | 723 | 723 | 723 |

| PDB annotation | INK4C; CELL CYCLE INHIBITOR, P18INK4C, TUMOR, SUPPRESSOR, CYCLIN-2 DEPENDENT KINASE, HORMONE/GROWTH FACTOR | HORMONE/GROWTH FACTOR P18- DNGC; CELL CYCLE NHBITOR, P18INKGC, THOMOR, SUPPRESSOR, CYCLIN-2 DEPENDENT KINASE, HORMONE/GROWTH FACTOR | CELL CYCLE INHIBITOR P18- INK4C(INK6); CELL CYCLE INHIBITOR, P18-INK4C(INK6), ANKYRIN REPEAT, 2 CDK 4/6 INHIBITOR. | CELL CYCLE INHIBITOR P18- INKAC(INK6); CELL CYCLE INHIBITOR, P18-INKAC(INK6), ANKYRIN REPEAT, 2 CDK 4/6 INHIBITOR | TRANSCRIPTION FACTOR P65; P50D; TRANSCRIPTION FACTOR, IKBANFKB COMPLEX | TRANSCRIPTION FACTOR P65; P50D; TRANSCRIPTION FACTOR, IKBANFKB COMPLEX | TRANSCRIPTION FACTOR P65, P50D; TRANSCRIPTION FACTOR, IKBANFKB COMPLEX | TRANSCRIPTION FACTOR P65, P50D; TRANSCRIPTION FACTOR, IKBANFKB COMPLEX | COMPLEX (TRANSCRIPTION REGIANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION REGIANK REPEAT) COMPLEX |
|----------------|---|---|--|---|---|--|---|---|--|--|
| Coumpound | KINASE 6 INHIBITOR; CHAIN: A; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B; | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; 1- KAPPA-B-ALPHA; CHAIN: D; | NF-KAPPA-B P65 SUBUNIT: CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; 1- KAPPA-B-AL,PHA; CHAIN: D; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA; CHAIN: D; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NP-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA; CHAIN: D; | NF-KAPPA-B P65, CHAIN: A, C, NF-KAPPA-B P50, CHAIN: B, D, I-KAPPA-B-ALPHA; CHAIN: E, F. | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: |
| SeqFold | | | | | | 10:19 | | | | |
| PMF | | 0.88 | 0.35 | 0.99 | _ | | 0.95 | 0.43 | 0.65 | - |
| Verify | | 0.32 | 0.07 | 0.15 | 0.13 | | 0.37 | -0.02 | 90.0 | 0.31 |
| PSI- BLAST | | 1.80E-26 | 1.80E-28 | 1.80E-33 | 1.80E-43 | 1.80E-43 | 3.60E-36 | 1.10E-28 | 5.40E-30 | 9.00E-44 |
| End | | 234 | 284 | 191 | 174 | 208 | 229 | 280 | 288 | 174 |
| Start AA | | 73 | 107 | 9 | 7 | 2 | 35 | 89 | 136 | .2 |
| Chain | | ∢ | < | ∢ | Δ | Ω | Д | Ω | ш | ш |
| 808 10 | | 1bu9 | gii. | lihb | Likn | likn | likn | likn | g. | Jul |
| SEQ No ed | | 723 | 723 | | 723 | 723 | 723 | 723 | 723 | 723 |

| PDB annotation | (TRANSCRIPTION REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION REGIANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT) ANKYRN 2 REPEAT HEI IX | COMPLEX (TRANSCRIPTION REGIANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX | COMPLEX (INHIBITOR/NUCLEASE) COMPLEX (INHIBITOR/NUCLEASE), COMPLEX (IR-ANG), HYDROLASE 2 MOLECULAR RECOGNITION, EPITOPE MAPPING, LEUCINE-RICH 3 REPEATS | COMPLEX (NHIBITORNUCLEASE) COMPLEX (NHIBITORNUCLEASE) COMPLEX (RHAND) HYDROLASE 2 MOLECULAR RECOGNITION, BPITODE MAPPING, LEUCINE-RICH 3 REPEATS | COMPLEX (INHIBITORANGLEASE) COMPLEX (ROHBITORANGLEASE), COMPLEX (RI-ANG), HYDROLASE 2 MOLECULAR RECOGNITION, EPITOPE MAPPING, LEUCINE-RICH 3 REPEATS | COMPLEX (INHIBITORANGLEASE) COMPLEX (RHBITORANGLEASE), COMPLEX (RHANG), HYDROLASE 2 MOLECULAR RECOGNITION, EPITOPE MAPPING, LEUCINE-RICH 3 REPEATS | COMPLEX (INHIBITOR/NUCLEASE) COMPLEX (INHIBITOR/NUCLEASE), COMPLEX (IR-ANG), HYDROLASE 2 MOLECULAR RECOGNITION, EPITOPE MAPPING, LEUCINE-RICH 3 REPEATS |
|-----------------|--|---|--|---|--|--|--|---|
| Coumpound | B, D; I-KAPPA-B-ALPHA; CHAIN: E, F; | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: F. F. | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E, F; | RIBONUCLEASE INHIBITOR, CHAIN: A, D, ANGIOGENIN; CHAIN: B, E, | RIBONUCLEASE INHIBITOR; CHAIN: A. D. ANGIOGENIN; CHAIN: B, E; | RIBONUCLEASE INHIBITOR; CHAIN: A, D; ANGIOGENIN; CHAIN: B, E; | RIBONUCLEASE INHIBITOR; CHAIN: A, D; ANGIOGENIN; CHAIN: B, E; | RIBONUCLEASE INHIBITOR; CHAIN: A, D; ANGIOGENIN; CHAIN: B, E; |
| SeqFold | | | 59.74 | | | | 93.46 | |
| PMF | | - | | 0.07 | 0.16 | 0.55 | | _ |
| Verify score | | 0.49 | | -0.4 | -0.3 | -0.33 | | 0.15 |
| PSI- BLAST | | 5.40E-36 | 9.00E-44 | 1.30E-13 | 9.00E-17 | 2.60E-22 | 3.90E-36 | 9.10E-39 |
| End | | 229 | 246 | 369 | 577 | 597 | 558 | 376 |
| Start AA | | 34 | 36 | _ | 219 | 267 | 82 | 83 |
| Chain ID | | a | ш | V V | ⋖ | A | ¥ | ¥ |
| PDB ID | | 1mfi | Infi | la4y | la4y | la4y | la4y | 184y |
| SEQ No: | | 723 | 723 | 725 | 725 | 725 | 725 | 725 |

| | | | : | | | | | | | | | | | |
|------------------|---|--|---|---|---|---|---|---|---|--|---|---|---|--|
| PDB annotation | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP,RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP, RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP,RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP,RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP,RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP,RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP,RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP,RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP,RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP, RIBONUCLEOPROTEIN | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP,RIBONUCLEOPROTEIN | CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL ADHESION | CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL ADHESION | CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL |
| Coumpound | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | UZ RNA HAIRPIN IV; CHAIN: Q, R; UZ A'; CHAIN: A, C; UZ B''; CHAIN: B, D; | UZ RNA HAIRPIN IV; CHAIN: Q, R; UZ A'; CHAIN: A, C; UZ B"; CHAIN: B, D; | UZ RNA HAIRPIN IV; CHAIN: Q, R; UZ A'; CHAIN: A, C; UZ B"; CHAIN: B, D; | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | UZ RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D; | INTERNALIN B; CHAIN: A; | INTERNALIN B; CHAIN: A; | INTERNALIN B; CHAIN: A; |
| SeqFold score | | | | | | | | | | | | | | |
| PMF | 0.57 | 0.75 | 0.77 | 0.45 | 0.99 | 0.84 | 0.88 | 69:0 | 0.45 | 0.55 | 96.0 | 89.0 | - | - |
| Verify score | -0.02 | 90:0 | 0.12 | -0.33 | 0.22 | -0.06 | 0.24 | -0.04 | 0 | 0.05 | 0.27 | -0.09 | 0.02 | 0.12 |
| PSI- BLAST | 5.20E-27 | 1.30E-25 | 3.90E-19 | 6.50E-20 | 3.90E-29 | 1.20E-27 | 2.60E-25 | 3.90E-19 | 6.50E-20 | 9.10E-26 | 6.50E-29 | 1.60E-26 | 1.30E-24 | 5.40E-29 |
| End | 306 | 351 | 576 | 576 | 228 | 319 | 321 | 576 | 576 | 213 | 236 | 158 | 319 | 364 |
| Start | 134 | 203 | 430 | 454 | 68 | 134 | 203 | 430 | 454 | 82 | 8 | | 104 | 216 |
| Chain | A | 4 | V | ¥ | Y | ပ | υ · | ပ | ပ | ၁ | ပ | ¥ | 4 | ٧ |
| PDB ED 61 | 1a9n | 1a9n | 1a9n | 1a9n | 1a9n | 1a9n | la9n | la9n | la9n | la9n | 1a9n | 1406 | 140b | 140b |
| SEQ NO. | 725 | 725 | 725 | 222 | 725 | 725 | 725 | 222 | 725 | 725 | 725 | 722 | 725 | 725 |

| | | | _ | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----------------|----------|---|---|---|--------------------------------------|----------------------------|------------------------|--|--------------|---------------------|----------------------|----------------------------|------------------------|----------------------|-------------------------|---------------------|----------------------|----------------------------|------------------------|---|---------------------|----------------------|----------------------------|------------------------|-------------------------|-----------------------|---------------------|--|
| PDB annotation | ADHESION | CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL ADHESION | CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL ADHESION | CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL ADHESION | TRANSFERASE CRYSTAL STRIICTHE RAB | GERANYLGERANYLTRANSFERASE, | 2.0 A 2 RESOLUTION, N. | FURM YLMEI HIONINE, ALPHA SUBUNIT, BETA SUBUNIT | : | TRANSFERASE CRYSTAL | STRUCTURE, RAB | GERANYLGERANYLTRANSFERASE, | 2.0 A 2 RESOLUTION, N- | COUNT DETA STIDIBLE | SOBOINIT, BETA SOBOINIT | TRANSFERASE CRYSTAL | STRUCTURE, RAB | GERANYLGERANYLTRANSFERASE, | 2.0 A 2 RESOLUTION, N- | SUBUNIT, BETA SUBUNIT | TRANSFERASE CRYSTAL | STRUCTURE, RAB | GERANYLGERANYLTRANSFERASE, | 2.0 A 2 RESOLUTION, N- | FORMYLMETHIONINE, ALPHA | SUBUNII, BEIA SUBUNII | TRANSFERASE CRYSTAL | STRUCTURE, RAB GERANYLGERANYLTRANSFERASE, |
| Coumpound | | INTERNALIN B; CHAIN: A; | INTERNALIN B; CHAIN: A; | INTERNALIN B; CHAIN: A; | RAB GFRANYI GERANYI TRANSF | ERASE ALPHA SUBUNIT; | CHAIN: A, C; RAB | GEKANY LGEKANYLIKANSF ERASE BETA SUBUNIT; | CHAIN: B, D; | RAB | GERANYLGERANYLTRANSF | ERASE ALPHA SUBUNIT; | CHAIN: A. C. RAB | DO ASE DETA SUBINITA | CHAIN: B, D; | RAB | GERANYLGERANYLTRANSF | ERASE ALPHA SUBUNIT; | CERAIN: A, C; KAB | GERAIN ILGERAIN ILLIKAINSF ERASE BETA SUBUNIT; CHAIN: B. D. | RAB | GERANYLGERANYLTRANSF | ERASE ALPHA SUBUNIT; | CHAIN: A, C; RAB | GERANYLGERANYLTRANSF | CHAIN: B. D: | RAB | GERANYLGERANYLTRANSF ERASE ALPHA SUBUNIT; |
| SeqFold | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF score | | 0.4 | 0.92 | 0.34 | _ | | | | | 0.95 | | | | | | 96.0 | | | | | 0.22 | | | | | | 0.07 | |
| Verify score | | 0.04 | 0.18 | 0.09 | 0.12 | | | | | -0.23 | | | | | | 0.18 | | | | | 80.0 | | | | | | 0.07 | |
| PSI- BLAST | | 9.00E-28 | 5.40E-24 | 1.10E-21 | 3.60E-13 | | | | | 5.40E-13 | | | | | | 9.00E-13 | | | | | 1.80E-13 | | | | | | 7.20E-09 | |
| End AA | | 406 | 991 | 965 | 301 | | | | | 346 | | : | | | | 369 | | | | | 533 | | | | | | 109 | |
| Start AA | | 242 | 32 | 415 | 216 | | | | | 246 | | | | | | 268 | | | | | 428 | | | | | | 475 | |
| Chain ID | | ٧ | ٧ | ¥. | ¥ | | | | | Ą | | | | | | A | | | | | ٧ | | | | | | ٧ | |
| EQB CD | | 1406 | 140b | 1d0b | 1dce | | | | | ldce | | | | | | 1dce | | | | | Ide | | | | | | Ide | |
| SEQ B B S | | 725 | 222 | 725 | 725 | | | | | 725 | | | | | | 725 | | | | | 725 | | | | | | 725 | |

| | | r | | | | | | | , |
|------------------|---|---|--|--|--|--|---|---|---|
| PDB annotation | 2.0 A 2 RESOLUTION, N- FORMYLMETHIONINE, ALPHA SUBUNIT, BETA SUBUNIT | TRANSFERASE CRYSTAL STRUCTURE, RAB ERANYLICHANYLIRANSFERASE, 2.0 A 2 RESOLUTION, N- FORMYLAEGHIONINE, ALPHA SUBUNIT, BETA SUBUNIT | CONTRACTILE PROTEIN LEUCINE- RICH REPEAT, BETA-BETA-ALPHA CYLINDER, DYNEIN, 2 CHLAMYDOMONAS, FLAGELLA | CONTRACTILE PROTEIN LEUCINE- RICH REPEAT, BETA-BETA-ALPHA CYLINDER, DYNEIN, 2 CHLAMYDOMONAS, FLAGELLA | CONTRACTILE PROTEIN LEUCINE- RICH REPEAT, BETA-BETA-ALPHA CYLINDER, DYNEIN, 2 CHLAMYDOMONAS, FLAGELLA | CONTRACTILE PROTEIN LEUCINE- RICH REPEAT, BETA-BETA-ALPHA CYLINDER, DYNEIN, 2 CHLAMYDOMONAS, FLAGELLA | CONTRACTILE PROTEIN LEUCINE- RICH REPEAT, BETA-BETA-ALPHA CYLINDER, DYNEIN, 2 CHI AMYDOMONAS, FLAGELLA | LIGASE CYCLIN A/CDK2- ASSOCIA/TED PROTEIN PS; CYCLIN A/CDK2-ASSOCIA/TED PROTEIN P19; SKP1, SKP2, F-BOX, LRR, LEUCINE- SKP1, SKP2, F-BOX, LRR, LEUCINE- TOWN PROTEIN LIGASE | LIGASE CYCLIN A/CDK2- ASSOCIATED PROTEIN P45; CYCLIN A/CDK2-ASSOCIATED PROTEIN P19; SKP1, SKP2, F-BOX, LRR, LEUCINE- |
| Coumpound | CHAIN: A, C; RAB GERANYLGERANYLTRANSF ERASE BETA SUBUNIT; CHAIN: B, D; | RAB BERNYLGERANYLTRANSF ERASE ALPHA SUBUNIT; CHAIN: A, C, RAB GERANYLGERANYLTRANSF ERASE BETA SUBUNIT; CHAIN: B, D; | OUTER ARM DYNEIN; CHAIN: A; | OUTER ARM DYNEIN; CHAIN: A: | OUTER ARM DYNEIN; CHAIN: A; | OUTER ARM DYNEIN; CHAIN: A; | OUTER ARM DYNEIN; CHAIN: A; | SKP2; CHAIN: A, C, E, G, I, K, M, O; SKP1; CHAIN: B, D, F, H, I, L, N, P; | SKP2; CHAIN: A, C, E, G, I, K, M, O; SKP1; CHAIN: B, D, F, H, J, L, N, P, |
| SeqFold score | | | | | | | | | |
| PMF | | 0.95 | 0.21 | 0.94 | 0.12 | 0.52 | 0.75 | 0.04 | 0.09 |
| Verify score | | 0.3 | -0.34 | -0.36 | -0.73 | -0.47 | -0.79 | 0.02 | -0.35 |
| PSI- BLAST | | 1.30E-13 | 3.60E-13 | 1.10E-14 | 7.20E-13 | 1.30E-13 | 3.90E-26 | 3.60E-07 | 1.30E-09 |
| End AA | | 170 | 140 | 324 | 346 | 164 | 213 | 172 | 575 |
| Start | | 09 | 17 | 210 | 232 | 02 | 83 | _ | 264 |
| Chain D | | ∢ | ٧ | ٧ | ٧ | ¥ | V | V | A |
| 808 CI | | Idce | 6spi | 1ds9 | 1ds9 | 1ds9 | 6sp1 | Ifqv | lfqv |
| SEQ BO | | 227 | 725 | 725 | 725 | 725 | 725 | 725 | 725 |

| PDB annotation | RICH RÉPEAT, SCF, UBIQUITIN, 2 E3, UBIQUITIN PROTEIN LIGASE | LIGASE CYCLIN A/CDK2- ASSOCIATED PROTEIN P45; CYCLIN A/CDK2-ASSOCIATED PROTEIN P19; | SKP1, SKP2, F-BOX, LRR, LEUCINE- RICH REPEAT, SCF, UBIQUITIN, 2 E3, UBIOUITIN PROTEIN LIGASE | LIGASE CYCLIN AYCDK2- ASSOCIATED P45; CYCLIN AYCDK2- ASSOCIATED P19; SKP1, SKP2, F-BOX, LRKS, LEUCINE-RICH REPEATS, SCP, 2 UBIQUITIN, E3, UBIQUITIN PROTEIN LIGASE | LIGASE CYCLIN AVDK2. ASSOCIATED P45, CYCLIN AVDK2. ASSOCIATED P19, SKP1, SKP2, F-BOX, LRRS, LEUCINE-RICH REPEATS, SCP, 2 UBIQUITIN, E3, UBIQUITIN PROTEIN LIGASE | LIGASE CYCLIN A/CDK2- ASSOCIATED P45; CYCLIN A/CDK2- ASSOCIATED P19; SKP1, SKP2, F-BOX, LRKS, LEUCINE-RUCH REPEATS, SCF, 2 UBIQUITIN, ES, UBIQUITIN PROTEIN LIGASU | TRANSCRITTION RAILP, RANGAP, GTRASE-ACTIVATING PROTEIN POR SENI, GTRASE-ACTIVA, TING PROTEIN, GAP, RAAIP, RANGAP, LRR, LEUCINE, 2 RCIE REPEAT PROTEIN, TWINNING, HEMIHEDRAL TWINNING, JARGOHEDRAL | ACETYLATION RNASE INHIBITOR, RIBONUCLEASEANGIOGENIN INHIBITOR ACETYLATION, LEUCINE- RICH REPEATS | ACETYLATION RNASE INHIBITOR, RIBONUCLEASE/ANGIOGENIN INHIBITOR ACETYLATION, LEUCINE- |
|------------------|--|---|--|---|--|---|---|---|--|
| Coumpound | | SKP2; CHAIN: A, C, E, G, I, K, M, O; SKP1; CHAIN: B, D, F, H, J, L, N, P; | | SKP2; CHAIN: A, C; SKP1; CHAIN: B, D; | SKP2; CHAIN: A, C; SKP1; CHAIN: B, D; | SKP2; CHAIN: A, C; SKP1; CHAIN: B, D; | GTPASE-ACTIVATING PROTEIN RNAI_SCHPO, CHAIN: A, B; | RIBONUCLEASE INHIBITOR; CHAIN: NULL; | RIBONUCLEASE INHIBITOR; CHAIN: NULL; |
| SeqFold score | | | | | | | | | |
| PMF | | 90'0 | | 0.11 | 0.27 | 0.31 | 0.04 | 0.22 | 0.87 |
| Verify score | | -0.06 | | 60.0- | -0.12 | -0.14 | -0.22 | -0.07 | -0.26 |
| PSI- BLAST | | 1.00E-16 | | 3.60E-11 | 7.80E-19 | 6.50E-40 | 1.30E-09 | 1.10E-19 | 5.40E-21 |
| End | | 253 | | 453 | 577 | 338 | 431 | 498 | 292 |
| Start AA | | . 84 | | 244 | 401 | 68 | 211 | 110 | 239 |
| Chain D | | ¥ | | ¥ | ¥ | V | Y | | |
| PDB CD | | Ifqv | | 162 | 1162 | 162 | lyrg | 2bnh | 2bnh |
| SEQ NO: | | 725 | | 725 | 222 | 725 | 725 | 725 | 725 |

| PDB annotation | RICH REPEATS | ACE I TATION KNASE INHIBITOK, RIBONUCLEASEANGIOGENIN INHIBITOR ACETYLATION, LEUCINE- RICH REPEATS | ACETYLATION RNASE INHIBITOR, RIBONUCLEASE/ANGIOGENIN INHIBITOR ACETYLATION, LEUCINE- RICH REPEATS | COMPLEX (TRANSCRIPTION REGILATIONIDIA) GABPALPHA; GABPBETA1; COMPLEX TRANSCRIPTION | REGULATION/DNA), DNA-BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN. | ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR | COMPLEX (TRANSCRIPTION REGULATION/DNA) GABPALPHA; | GABPBETA1; COMPLEX | REGULATION/DNA), DNA-BINDING, 2 | NUCLEAR PROTEIN, ETS DOMAIN, | ANKTKIN KEPEALS, IKANSCKIPTION 3 FACTOR | COMPLEX (TRANSCRIPTION REGIT ATTOM/DNA) GARPAT PHA: | GABPBETAI: COMPLEX | (TRANSCRIPTION REGINAL SINDING 2 | NUCLEAR PROTEIN, ETS DOMAIN, | ANKYRIN REPEATS, TRANSCRIPTION | COMPLEX (TRANSCRIPTION | REGULATION/DNA) GABPALPHA; | (TRANSCRIPTION | REGULATION/DNA), DNA-BINDING, 2 | NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION |
|---|-----------------------------|---|--|---|---|--|---|-------------------------|---------------------------------|------------------------------|--|---|-------------------------|----------------------------------|------------------------------|--------------------------------|------------------------|----------------------------|-----------------------------|---------------------------------|--|
| Coumpound | PIPOSITION EACE BUILDINGON. | KIBONUCLEASE INHIBITUK; CHAIN: NULL; | RIBONUCLEASE INHIBITOR; CHAIN: NULL; | GA BINDING PROTEIN ALPHA; CHAIN: A; GA BINDING PROTEIN BETA 1; CHAIN: R: DNA: CHAIN: D. E: | | | GA BINDING PROTEIN ALPHA: CHAIN: A: GA | BINDING PROTEIN BETA 1; | CHAIN, B, DINA, CHAIN, D, E, | | | GA BINDING PROTEIN | BINDING PROTEIN BETA 1; | CHAIN: B; DNA; CHAIN: D, E; | | | GA BINDING PROTEIN | ALPHA; CHAIN: A; GA | CHAIN: B. DNA: CHAIN: D. E. | | - |
| SeqFold | | | 90.38 | | | | | | | | | 53.5 | | | | | | | | | |
| PMF | | | | -0.03 | | | 0.29 | | | | | | | | | | 0.72 | | | | |
| Verify score | 100 | 26.93 | | 0.12 | | | 61.0 | | | | | - | | | | | 0.32 | | | | |
| PSI- BLAST | 0, 100 | 1.80E-19 | 1.10E-19 | 3.60E-32 | | | 1.30E-35 | | | | | 1.30E-35 | | | | | 1.60E-31 | | | | |
| End | , | 8 | 558 | 145 | | | .167 | | | | | 179 | | | | | 203 | | | | |
| Start | | ۹ | 82 | 2 | *** | | 23 | | | | | 27 | | | | | 55 | | | | |
| Chain | | | | щ | | | æ | | | | | В | | | | | В | | | | |
| PDB DD | | 7puh | 2bnh | Іамс | | | lawc | | | | | lawc | | | | | lawc | | | | |
| SE SE SE SE SE SE SE SE SE SE SE SE SE S | i | 52 | 725 | 728 | | | 728 | | | | | 728 | | | | | 728 | _ | | | |

| PDB annotation | 3 FACTOR | HORMONE/GROWTH FACTOR P18- INK4C; CELL CYCLE INHIBITOR, | PISINK4C, TUMOR, SUPPRESSOR, | CYCLIN- 2 DEPENDENT KINASE, | HORMONE/GROWTH FACTOR P18- | INK4C; CELL CYCLE INHIBITOR, | P18INK4C, TUMOR, SUPPRESSOR, | CYCLIN-2 DEPENDENT KINASE, | HORMONE/GROWTH FACTOR P18. | INK4C: CELL CYCLE INHIBITOR. | PI8INK4C, TUMOR, SUPPRESSOR, | CYCLIN- 2 DEPENDENT KINASE, | HORMONE/GROWTH FACTOR | CELL CYCLE INHIBITOR P18- | INK4C(INK6); CELL CYCLE | INHIBITOR, P18-INK4C(INK6), | ANKYRIN REPEAT, 2 CDK 4/6 | INHIBITOR | TRANSCRIPTION FACTOR P65; P50D; | IKANSCKIPTION FACTOR, IKBINFKB | COMPLEX | | TRANSCRIPTION FACTOR P65; P50D; | COMPLEX | | COMPLEX (TRANSCRIPTION | REG/ANK REPEAT) COMPLEX | (TRANSCRIPTION REGULATION/ANK | REPEAT), ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION | REG/ANK REPEAT) COMPLEX | (TRANSCRIPTION REGULATION/ANK | REPEAT), ANKYRIN 2 REPEAT HELIX | COMPLEX (TRANSCRIPTION | REG/ANK REPEAT) COMPLEX | (TRANSCRIPTION REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX |
|------------------|----------|--|------------------------------|-----------------------------|----------------------------|------------------------------|------------------------------|----------------------------|----------------------------|------------------------------|------------------------------|-----------------------------|-----------------------|---------------------------|-------------------------|-----------------------------|---------------------------|---|---------------------------------|--------------------------------|------------------------|------------------------------|---------------------------------|-----------------------|--------------------------|---------------------------|---------------------------|-------------------------------|---------------------------------|---------------------------|---------------------------|-------------------------------|---------------------------------|---------------------------|---------------------------|---|
| Coumpound | | CYCLIN-DEPENDENT KINASE 6 INHIBITOR; | CHAIN: A; | | CYCLIN-DEPENDENT | KINASE 6 INHIBITOR; | ĆHAIN: A; | | CVCI IN-DEPENDENT | KINASE 6 INHIBITOR: | CHAIN: A; | | | CYCLIN-DEPENDENT | KINASE 6 INHIBITOR; | CHAIN: A, B; | | min at any and at the state of | Oliver A. N. V. V. V. P. C. | CHAIN: A; NF-KAFFA-B F30D | VAPPA B. AI PHA: C; I- | NALL A-B-ALLI IIA, CHAIN. D. | CHAIN A: NF-KAPPA-R P50D | SUBUNIT; CHAIN: C; I- | KAPPA-B-ALPHA; CHAIN: D; | NF-KAPPA-B P65, CHAIN: A, | C; NF-KAPPA-B P50; CHAIN: | B, D; I-KAPPA-B-ALPHA; | CHAIN: E, F; | NF-KAPPA-B P65; CHAIN: A, | C; NF-KAPPA-B P50; CHAIN: | B, D; I-KAPPA-B-ALPHA; | CHAIN: E, F; | NF-KAPPA-B P65; CHAIN: A, | C; NF-KAPPA-B P50; CHAIN: | B, D; I-KAPPA-B-ALPHA; CHAIN: E, F; |
| SeqFold score | | | | | | | | | I | | | | | | | | | | | | _ | | | | | | | | | | | | | | | |
| PMF | | 10:0 | | | 60.0 | | | | 5 15 | : | | | | 0.41 | | | | | P.74 | | | | 570 | | | 0.22 | | | | 0.36 | | | | 60.0 | | |
| Verify score | | 0.33 | | | 0.28 | | | | 20.00 | | | | | 0.25 | | | | , | ci.o | | | 200 | 77.0 | | | 0.24 | | | | 9.16 | | | | 0.03 | | |
| PSI- BLAST | | 1.80E-29 | | | 1.80E-29 | | | | 1.40E-27 | | | | | 3.60E-29 | | | | 2000 | 7:00E-37 | | | 1 000 30 | 1.80E-32 | | | 9.00E-37 | | | | 5.40E-32 | | | | 1.30E-26 | | |
| End | | <u> </u> | | | 150 | | | | 250 | | | | | 166 | | | | 671 | 70 | | | 200 | 841 | | | 162 | | | | 198 | | | | 245 | | |
| Start AA | | 23 | | | 2 | | | | 16 | | | | | 23 | | | | 5 | 2 | | | 10 | 9 | | | 12 | | | | 1 | _ | | | 8 | | |
| Chain D | | ∢ | | | Ą | | | | \ \ | | | | | ۷ | | | | - | ۹. | | | 6 | 2 | | | ш | | | | m) | | | | ш | | |
| PDB DD | | 1bu9 | | | 1bu9 | | | | 1hu9 | | | | | 4 <u>1</u> | | | | | 1 | | | 1 | 2 | | | III. | _ | | | Ħ | | • |] | E E | | |
| SEQ NO: | | 22 | | _ | 728 | | | | 728 | | | | | 728 | | | | 120 | ş | _ | | 130 | 3 | | | 728 | _ | _ | | 728 | | | 1 | 23 | | |

| PDB annotation | COMPLEX (TRANSCRIPTION REGIANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT), ANK YRIN 2 REPEAT HELIX | PHOSPHOTRIESTERASE PHOSPHOTRIESTERASE, HYPOTHETICAL PROTEIN | SI RNA-BINDING DOMAIN POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE, SI RNA-BINDING DOMAIN, POLYNUCLEOTIDE PHOSPHORYLASE 2 (PNPASE) | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX |
|------------------|--|---|---|---|---|---|---|--|---|
| Coumpound | NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I-KAPPA-B-ALPHA; CHAIN: E, F; | PHOSPHOTRIESTERASE HOMOLOGY PROTEIN; CHAIN: A, B; | PNPASE; CHAIN: NULL; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B.C: | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSK ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN: CHAIN: C, F, G; |
| SeqFold score | | | | | 81.11 | | | | |
| PMF | 0.03 | 69:0 | - | 0.82 | | - | 6.0 | 96:0 | _ |
| Verify score | 90:0 | 0.37 | 0.13 | 80:0 | | -0.04 | -0.33 | 90:0 | 0.27 |
| PSI- BLAST | 5.40E-29 | 3.90E-07 | 5.40E-23 | 1.10E-26 | 7.80E-45 | 7.80E-45 | 6.50E-41 | 1.80E-43 | 3.60E-46 |
| End | 253 | 208 | 618 | 217 | 443 | 469 | 498 | 217 | 245 |
| Start AA | . 88 | 74 | 540 | 137 | 361 | 389 | 417 | 136 | 164 |
| Chain D | ш | 4 | | < | < | V | ¥ | ပ | ပ |
| PDB ID | Jul | 1666 | lsro | lalh | lalh | lalh | lalh | 1те у | Ime y |
| S a S | 728 | 729 | 731 | 736 | 736 | 736 | 736 | 736 | 736 |

| | , | | | | | | | | | _ | | | | | | | | | | | | | _ | | _ | | | | | | _ | | | |
|--|-------------------|--------------------------------|--------------------------------|----------------------------|--------------------------------|-----------------------|--------------------------------|-------------------|--------------------------------|-----------------------|--------------------------------|----------------------------|------------------------------|-----------------------|--------------------------------|----------------------------|-------------------|-------------------------------|-------------------------------|---------------------------|-------------------|--------------------------------|-----------------------|--------------------------------|----------------------------|--------------------------------|-----------------------|--------------------------------|----------------------------|-------------------|--------------------------------|-----------------------|--------------------------------|---|
| PDB annotation | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | COMPLEY (7NC FINGER/DNA) 2NC | FINGER PROTFIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC | PATER ACTION PROTEIN DESIGN 2 | CRYSTAL STRUCTURE COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRISIAL SIRUCIUME, COMPLEX (ZINC FINGER/DNA) |
| Coumpound | | DNA; CHAIN: A, B, D, E; | PROTEIN; CHAIN: C, F, G; | | DNA; CHAIN: A. B. D. E. | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C. F, G; | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | DNA CHAIN A B D E. | CONSENSIS ZINC FINGER | PROTEIN: CHAIN: C. F. G. | | | DNA; CHAIN: A, B, D, E; | DECTER: CLANS C. P. C. | FNOIBIN, CIPAIN: C, F, G, | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | DNA: CHAIN: A B D E | CONSENSUS ZINC FINGER | PROTEIN: CHAIN: C, F, G; | • | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | |
| SeqFold | | | | | | | | | | | | | | | | | | | | | | 104.61 | | | | | | | | | | | | |
| PMF | | _ | | | _ | | | | _ | | | | - | | | _ | | _ | | | | | | | | - | | | | | - | | | |
| Verify score | | 0.41 | | | 0.19 | | | | 0.38 | | | | 92.0 | | | | | 0.46 | | | | | | | | 0.44 | | | | | 0.05 | | | |
| PSI- BLAST | | 9.00E-48 | | | 7.20E-49 | | | | 9.00E-51 | | | | 7.20F-51 | | | | | 3.60E-50 | | | | 7.20E-51 | | | | 9.00E-50 | | | | | 3.60E-50 | | | |
| End | | 273 | | | 301 | | | | 357 | | | | 385 | | | | | 413 | | | | 414 | | | | 14 | | | | | 469 | | | |
| Start | | 192 | | | 220 | | | | 276 | | | | 304 | | | | | 332 | | | | 332 | | | | 360 | | | | | 388 | | | |
| Chain ID | | 2 | | | ပ | | | | 2 | | | | c | | | | | ပ | | | | ပ | | | | o | | | | | ပ | | | |
| PDB ID | | 1me | | | line I | > | | | lme | ^ | _ | | and a | > | | | - | ıl , | _ | | | e e | > | | | Ime | ^ | | | | Ine : | > | | |
| SEQ B SO SO SO SO SO SO SO SO SO SO SO SO SO | | 736 | | | 736 | | | | 736 | | | | 736 | | | | | 736 | | | | 736 | | | | 736 | | | | | 736 | | | |

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|------------------|---|---|--|---|--|--|--|
| PDB annotation | COMPLEX (ZINC FINGER/DINA) ZINC FINGER, PROTEIN-DINA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DINA) | COMPLEX (TRANSCRIPTION REGULATIONIONA) COMPLEX (TRANSCRIPTION REGULATIONIONA), RNA REGULATIONIONA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONNA) COMPLEX (TRANSCRIPTION REGULATIONONA), RNA REGULATIONONA), RNA POLYMEASSE III, 2 TRANSCRIPTION MITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONINA) COMPLEX (TRANSCRIPTION) REGULATIONINA), RNA REGULATIONINA), RNA POLYMERASE III, STRANSCRIPTION NITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONINA) COMPLEX (TRANSCRIPTION REGULATIONINA), RNA REGULATIONINA), RNA POLYMEASER III, STRANSCRIPTION NITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONINA) COMPLEX (TRANSCRIPTION REGULATIONINA), RNA REGULATIONINA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FRIGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-YANG 1; TRANSCRIPTION INITIATION, INITIATION, INITIATIOR ELEMENT, YY I. ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECGGNITION, 3 COMPLEX |
| Coumpound | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA: CHAIN: A, B; |
| SeqFold score | | | | 112.4 | | · | |
| PMF | | 0.33 | | | 0.95 | 0.92 | 0.19 |
| Verify | 0.1 | 0.09 | 0.04 | | -0.11 | -0.04 | 0.01 |
| PSI- BLAST | 1.80E-50 | I.40E-34 | 1.105-36 | 2.60E-79 | 3.60E-38 | 1.60E-35 | 5.40E-29 |
| End | 497 | 282 | 338 | 4 | 479 | 499 | 217 |
| Start AA | 416 | 137 | 163 | 276 | 333 | 361 | III |
| Chain D | 2 | ¥ | ¥ | ¥ | ¥ | ¥ | ပ |
| PDB DD | Ime y | 1146 | 1166 | 911 | 1146 | Itf6 | 1ubd |
| S e S | 736 | 736 | 736 | 736 | 736 | 736 | 736 |

| PDB annotation | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REQUILATIONDAM YING-YANG 1; TRANSCRIPTON INITIATION, INITIATIOR ELEMBAT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULT/DIONDA/J YING-YANG 1; TRANSCRIPTION INTHATION, MITHATOR ELEMENT, YYI, ZENC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX TRANSCRIPTION REGIT ACTIONDAA | COMPLEX (TRANSCRIPTION REGULET (TONONA) YING-YANG 1; TRANSCRIPTION MITHATION INITATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX TRANSCRIPTION REGIT A, TONONA | COMPLEX (TRANSCREPTON REGULATIONONA) YING-YANG I; TRANSCREPTON MITHATION, MITHATOR ELEMENT, YYI, ZENC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITON, 3 COMPLEX RECORMITON, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATIONONA) YING-YANG 1; TRANSCRIPTION MITHATION, MITHATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECORMITON, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN |
|------------------|--------------------------------|---|---|---|---|--|--|
| Coumpound | | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAM: C; ADENO- ASSOCIATED VIRUS PS INTIATOR ELEMENT DNA; CHAIN: A, B; | YYI, CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; |
| SeqFold score | | | | | | 89.47 | |
| PMF | | - * | - | _ | - | | _ |
| Verify | | 0.03 | 0.18 | 0.11 | 0.1 | | 10:0 |
| PSI- BLAST | | 1.00E-56 | 1.30E-55 | 1.20E-57 | 3.90E-57 | 3.90E-57 | 2.60E-56 |
| End | | 273 | 329 | 358 | 385 | 414 | 469 |
| Start AA | | 162 | 218 | 246 | 274 | 304 | 359 |
| Chain | | ပ | U | ပ | U | U | U |
| E G | | Pan Pan Pan Pan Pan Pan Pan Pan Pan Pan | Jubd | Jubd | Pqn | Jubd | Jubd |
| ğa ş | - | 736 | 736 | 736 | 736 | 736 | 736 |

| | | | | | | | | | | | | | | _ | | | | | | | | | | _ | _ | | |
|------------------|---|---|-------------------------------|---|--|---------------------------|---|------------------------|------------------------|--------------------------|--------------------------------|-----------------------------|------------------------|--|------------------------------------|----------------------------|----------------------|---------------------------|---|----------------------|---------------------------|------------------------------------|--|---------------------------|------------------------------------|--|---|
| PDB annotation | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG I; TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YYI, ZINC2 | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-YANG 1; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION | TRANSCRIPTION INTIATION. | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | ON THE PRINCIPLE OF THE | PROTEIN/DNA) FIVE-FINGER GLI: GLI. | ZINC FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/UNA) FIVE-FINGER GLI; GLI, ZINC FINGER COMPT EX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, |
| Coumpound | | YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; | CHAIN: A, B; | | YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | YY1; CHAIN: C; ADENO- | NITIATOR ELEMENT DNA: | CHAIN: A, B; | | | This raises another of the | CHAIN: A: DNA: CHAIN: C. | D; | | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, | î. | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, | ä | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, | á | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | - | | | 96.0 | | | | 66'0 | | | | | | _ | | | | | | _ | | | _ | | | |
| Verify score | | 0 | | | -0.18 | | | | -0.04 | | | | | | 7.0 | | | 0.38 | | | 0.22 | | | 0.03 | | | 0.58 |
| PSI- BLAST | | 1.80E-34 | | | 3.90E-51 | | | | 3.60E-34 | | | | - | 0 000 | . 8C-500.7 | | | 1.80E-34 | | | 2.60E-70 | | | 5.20E-74 | | | 1.30E-73 |
| End AA | | 469 | | | 497 | | | | 497 | | | | | 27.6 | C/7 | | | 300 | | | 303 | | | 329 | | | 387 |
| Start | | 368 | | | 386 | | | | 396 | | | | | 5 | DCT . | | | 164 | | | 164 | | | 192 | | | 249 |
| Chain | | ပ | | | O | | | | ပ | | | | | | < | | | ٧ | | | ٧ | | | 4 | | | ∢ |
| 108 CI | | lubd | | | lubd | | | | lubd | | | | | | 7811 1187 | | | 2gli | | | 2gli | | | 2gli | | | 2gli |
| S a S | | 736 | | | 736 | | | | 736 | | | | | 1 | 8 | | | 736 | | | 736 | | | 736 | | | 736 |

| PDB annotation | ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLJ; GLJ, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | CATALYTIC ANTIBODY CATALYTIC | COMPLEX (AVIIBODY/PETIDE) POLYSPECIFICITY, CROSS REACTIVITY, FAB-PRAGMENT, PEPTIDE, 2 HIV-I, COMPLEX (ANTIBODY/PEPTIDE) | CONTRACTILE PROTEIN IMMUNOGLOBULIN FOLD, BETA BARREL | ANTIBODY FAB FRAGMENT ANTIBODY FAB FRAGMENT | |
|-----------------|--|---|--|--|---|---|--|------------------------------|---|--|---|-----------------------|
| Coumpound | D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A: DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | 29G11 FAB; CHAIN: L, H; | ANTIBODY (CB 4.1); CHAIN: A, B; PEPTIDE; CHAIN: C; | TELOKIN; CHAIN: A | ANTI-ANTI-IDIOTYPE GH1002 FAB FRAGMENT; CHAIN: L. H | T LYMPHOCYTE ADHESION |
| SeqFold | | 92.84 | | | | | | 55.38 | 55.09 | | 57.41 | 69.87 |
| PMF | | | - | _ | _ | | 0.05 | | | -0.12 | | |
| Verify score | | | 90:0- | 90:00 | 0.03 | 0.19 | -0.23 | | | 0.19 | | |
| PSI- BLAST | | 5.20E-74 | 2.60E-72 | 3.60E-33 | 2.60E-68 | 3.60E-34 | 5.40E-29 | 7.20E-05 | 3.60E-05 | 1.60E-17 | 0.0054 | 9.10E-18 |
| End | | 387 | 471 | 468 | 499 | 496 | 216 | 230 | 230 | 212 | 230 | 213 |
| Start AA | | 250 | 305 | 340 | 360 | 368 | 89 | 20 | 19 | 126 | 61 | 24 |
| Chain TD | | ¥ | ¥ | V | ٧ | ¥ | Ą | L | ٧ | A | ı. | |
| PDB UD | | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 1a0q | 1bog | 1fhg | 1ghf | lhnf |
| SEQ No de | | 736 | 736 | 736 | 736 | 736 | 736 | 741 | 741 | 741 | 741 | 741 |

| PDB annotation | | | | | COMPLEXE COMPLIANT OF THE COMPLEXE COMPLEX COMPLEX COMPLEX COMPLEX COMPLEX COMPLEXE SERVES 2 PROTEIN A COMPLEXED WITH FABIR4.1, BORNELIA BURGDOKPERI 3 STRAIN BIRRELIA BURGDOKPERI 3 STRAIN BURNELIA BURGDOKPERI 3 STRAIN B | | | CELL ADHESION PROTEIN NCAM MODULE 2, CELL ADHESION, GUYCOPROTEIN, HEPARN-BINDING, GPI-ANCHOR, 2 NEURAL ADHESION MOLECULE, INAMONOGLOBULIN FOLD, HOMOPHILIC 3 BINDING, CELL ADHESION PROTEIN | LIGASE CYCLIN AČDIK2. ASSOCIATED PROTEIN P45, CYCLIN ACDIK2-ASSOCIATED PROTEIN P19, SKT1, SKT2, F-BOX, LRL, LEUCINE- RTCH REPEAT, SCF, UBIQUITIN, 2 E3, UBIQUITIN PROTEIN LIGASE |
|------------------|------------------------------------|---|--|---|--|---|---|---|--|
| Coumpound | GLYCOPROTEIN CD2 (HUMAN) 1HNF 3 | T LYMPHOCYTE ADHESION GLYCOPROTEIN CD2 (HUMAN) IHNF 3 | TLYMPHOCYTE ADHESION GLYCOPROTEIN CD2 (RAT) 1HNG 3 | T LYMPHOCYTE ADHESION GLYCOPROTEIN CD2 (RAT) IHNG 3 | FAB 1841; CRAIN: I., H: OUTER SURFACE PROTEIN A; CHAIN: O; | MUSCLE PROTEIN TITIN MODULE MS (CONNECTR) ITNM 3 TOMR, MINIMIZED A VERAGE STRUCTURE) ITNM 4 ITNM 58 | IMMUNOGLOBULIN IGG2A FAB FRAGMENT (CN1206) 2GFB 3 | NEURAL CELL ADHESION MOLECULE, LARGE ISOFORM; CHAIN: A; | SKP2; CHAIN: A, C, E, G, I, K, M, G, SKP1; CHAIN: B, D, F, H, J, L, N, P; |
| SeqFold score | | | 60.69 | | 55.92 | | 53.4 | | |
| PMF score | | 0.76 | | 0.35 | | 0.18 | | -0.18 | 0.92 |
| Verify score | | 60.0 | | 0.35 | | 0.00 | | 0 | -0.07 |
| PSI- BLAST | | 9.10E-18 | 2.60E-18 | 2.60E-18 | 0.0011 | 3.60E-14 | 3.60E-05 | 1.80E-09 | 2.60E-05 |
| End AA | | 661 | 217 | 210 | 230 | 213 | 230 | 8 8 | 81 |
| Start AA | | 28 | 25 | 29 | 19 | 131 | 61 | | 46 |
| Chain ID | | | A | Ą | ı | | ¥ | ∢ | 4 |
| EDB EL | | Jhf. | Ihng | Thng | losp | Imm I | 2gfb | 3nc m | 1fqv |
| SEQ No: | | 741 | 741 | 741 | 741 | 741 | 741 | 741 | 747 |

| PDB annotation | COMPLEX (DNA-BNDING PROTEINDNA) UPSTREAM STIMULATORY FACTOR I; USF, DNA BINDING, BASIC-HELIZ-LOOP-HELIX, LEUCINE ZIPPER, 2 TRANSCRIPTION FACTOR, COMPLEX (DNA-BINDING PROTEINDNA) | TRANSCRIPTION FACTOR P65; P50D; TRANSCRIPTION FACTOR, IKBNFKB COMPLEX | COMPLEX (TRANSCRIPTION FACTOR/DNA) NF-KB PS0, COMPLEX (TRANSCRIPTION FACTOR/DNA) | | HYDROLASE MALTOGENIC ALPHA AMYLASE, AMYLASE, GLYCOSIDE HYDROLASE, STARCH DEGRADATION | | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX |
|----------------|---|---|--|---|---|---|---|---|---|
| Coumpound | USF; CHAIN: A, B; DNA; CHAIN: C, D; | NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I- KAPPA-B-ALPHA; CHAIN: D; | NUCLEAR FACTOR KAPPA- B; CHAIN: A, B; KB SITE, DNA (5-D(TGAGAATTCCC)- 3'); CHAIN: C, D; | GLYCOSYLTRANSFERASE CYCLODEXTRIN GLUCANOTRANSFERASE (E.C.2.4.1.19) (CGTASE) ICYG | ALPHA-AMYLASE; CHAIN: A; | CHROMOSOMAL PROTEIN UBIQUITIN 1UBI 3 | QGSR ZINC FINGER PEPTIDE, CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE, CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B. C: | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; |
| SegFold | | | | | | | | | |
| PMF | 0.09 | 0.41 | 0.04 | 0.05 | 0.37 | 0.03 | 0.03 | 0.03 | 0.04 |
| Verify | -0.61 | 0.39 | -0.37 | -0.02 | 0.11 | -0.58 | -0.45 | -0.33 | -0.52 |
| PSI- BLAST | 0.0078 | 0.0013 | 0.0013 | 0.0016 | 0.0061 | 0.0065 | 3.60E-25 | 3.60E-24 | 1.40E-44 |
| End AA | 390 | 346 | 319 | 1059 | 196 | 1191 | 314 | 162 | 220 |
| Start | 353 | 243 | 234 | 932 | 854 | 1529 | 229 | 7.8 | 134 |
| Chain | 4 | ¥ | ٧ | | A | | A | ¥ | S |
| PDB | lan4 | lik | lnfk | lcyg | olpl | lubi | lalh | lalh | 1mc y |
| 8 a 8 | 750 | 750 | 750 | 754 | 754 | 754 | 756 | 756 | 756 |

| | | | | | | | | | | | | | | | | | | | | | | _ | | | _ | | | | | _ | | |
|----------------|-------------------|---|--|--------------------------------|---|-------------------|--------------------------------|------------------------------|----------------------------|-------------------|--------------------------------|-----------------------|--------------------------------|----------------------------|-----------------------------------|-----------------------|--------------------------------|----------------------------|-------------------|--------------------------------|----------------------|----------------------------|-------------------|--------------------------------|-----------------------|--------------------------------|----------------------------|-------------------|--------------------------------|-----------------------|---------------------------|-------------------|
| PDB annotation | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | INTERACTION PROTEIN DESIGN 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | COMPLEY (ZINC FINCED (DNIA) 2'BIC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, FROIEIN-DIA | COVETAL STRICTURE COMPLEY | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | CRYSTAL STRICTURE COMPLEX | (ZINC FINGER/DNA) |
| Coumpound | | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN: CHAIN: C, F, G; | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | | DNA; CHAIN: A, B, D, E; | PROTEIN CHAIN C. P. G. | 6 (1) | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | DNA: CHAIN A D D D. | CONSENSUS ZINC FINGER | PROTEIN: CHAIN: C. F. G. | | | DNA; CHAIN: A, B, D, E; | DECTENIO CHAIN OF G. | racially, challe, c, f, c, | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | | DNA; CHAIN: A, B, D, E, | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | |
| SeqFold | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF score | | 90:0 | | 0.28 | | _ | 0.12 | | | | -0.07 | | | | 0.17 | <u>.</u> | | | | 0.05 | | | | 0.07 | | | | | 61.0- | | | |
| Verify | | 9.0- | | -0.15 | | | -0.19 | | | | 90:0 | | | | 0.44 | ‡ | | | | 90.0 | | | | -0.3 | | | | | 90:0 | | | |
| PSI- BLAST | | 9.00E-44 | | 3.60E-42 | | | 1.10E-42 | | | | 3.60E-30 | | | | 1 905 40 | 1.00E-42 | | | | 5.40E-12 | | | | 9.00E-11 | | | | | 9.00E-11 | | | |
| End | | 284 | | 465 | | | 612 | | | | 627 | | | | 691 | 701 | | | | 130 | | | | 284 | | | | | 465 | | | |
| Start AA | | 193 | | 379 | | | 526 | | | | 555 | | | | - 1. | | | | | 163 | | | | 254 | | | | | 437 | | | |
| Chain | | ပ | | ပ | | | U | | | | ပ | | | | c | - ر | | | | o | | | | g | | | | | 9 | | | |
| PDB DD | | Jme y | | Jmc | >- | | lme : | _ | | | e E | > | | | 1me |) - - | | | | lie : | ` | | | lme | ^ | | | | Inc | ` | | |
| SEQ B B SE | | 756 | | 756 | | | 95/ | | | | 756 | | | | 75.6 | 3 | | | | 726 | | | | 756 | | | | | 756 | | | |

| PDB annotation | COMPLEX (TRANSCRIPTION REGILATION/DNA), FITH, 3S GENE, NMR, TRILA, PROTEIN, DNA, TRANSCRIPTION FACTOR, 3S RNA 2 GENE, DNA BINDING PROTEIN, ZINC FINGER, COMPLEX, | COMPLEX (TRANSCRIPTION REGILLATIONIONA) COMPLEX (TRANSCRIPTION) REGULATIONIONA), RNA REGULATIONIONA), RNA ROLYMARKSE II, 2 TRANSCRIPTION INTIATION, ZNC, ENGRR PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION) REGULATION/DNA), RNA REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION NITTATION, ZNC, FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONONA) YING-YANG I; TRANSCRIPTION INTHATION, INTILATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATIONONA) YING-YANG I; TRANSCRIPTION INTIATION, INTIATION B. ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATIONONA) YING-YANG; TRANSCRIPTION NITHATION, NITHATION, PINTATOR ELEMENT, YYI, 2MC2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX TRANSCRIPTION REGIT A TONDINA | COMPLEX (TRANSCRIPTION |
|-----------------|--|--|---|--|---|---|------------------------|
| Coumpound | TRANSCRIPTION FACTOR IIIA; CHADY: A; 58 RNA GENE; CHAIN: E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A. B: | YYI; CHAIN: C; ADENO. ASSOCIATED VIRUS P5 INTIATOR ELEMENT DNA; CHAIN: A, B; | YY1; CHAIN: C; ADENO- |
| SeqFold | | 69.84 | | | | | |
| PMF | 0.34 | | 0.11 | 0.11 | 0.23 | 0 | 0.01 |
| Verify score | -0.43 | | -0.18 | -0.77 | -0.21 | -0.72 | -0.53 |
| PSI- BLAST | 1.80E-15 | 1.40E-34 | 1.40E-34 | 1.30E-30 | 1.80E-27 | 1.80E-31 | 1.80E-30 |
| End | 432 | 282 | 302 | 253 | 436 | 278 | 8 |
| Start | 349 | 901 | 135 | 139 | 325 | | 85 |
| Chain D | ∢ | V | ¥ | v | ပ | ပ | ၁ |
| EDB CI | <u>a</u> | 題 | 941 | Iubd | Inbd | Jubd | lubd |
| SEQ No. ib | 756 | 756 | 952 | | 95/ | 756 | 756 |

| | | | | | | | | | | _ | |
|-----------------|--|--|---|--|---|--|--|---|---|-----------------|---|
| PDB annotation | REGULATION/DNA) YING-YANG I; TRANSCRIPTION MITHATION, INITATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DA) | TRANSCRIPTION REGULATION TRANSCRIPTION REGULATION, ADR.I. ZINC FINGER, NMR | TRANSCRIPTION REGULATION TRANSCRIPTION REGULATION, ADRI, ZINC FINGER, NMR | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | STRUCTURAL PROTEIN TWO REPEATS OF SPECTRIN, ALPHA HELICAL LINKER REGION, 2.2 TANDEM 3-HELIX COLED-COILS, STRUCTURAL PROTEIN | STRUCTURAL PROTEIN TWO REPEATS OF SPECTRIN, ALPHA HELICAL LINKER REGION, 22 TANDEM 3-HELIX COLED-COLLS, STRUCTURAL PROTEIN | CYTOSKELETON | SIGNALING PROTEIN DAPPI, PHISH, BAM35, PECKSTRIN, 3- PHOSPHOINOSITIDES, INOSITOL TETRAKISPHOSPHATE 2 SIGNAL TRANSDUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN ARF! GUANINE NUCLEOTIDE EXCHANGE FACTOR AND PH DOMAIN | | TRANSFERASE RECEPTOR TYROSINE KINASE, PROTEIN INTERACTION |
| Соитроипа | ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | ADRI; CHAIN: NULL; | ADR1; CHAIN: NULL; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ALPHA SPECTRIN; CHAIN: A, B, C; | ALPHA SPECTRIN; CHAIN: A, B, C; | BETA-SPECTRIN; 1DRO 6 CHAIN: NULL: 1DRO 7 | DUAL ADAPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | GRP1; CHAIN: A; | a contract of a | EPHA4 RECEPTOR TYROSINE KINASE; CHAIN: |
| SeqFold | | | | | | | | | | I | |
| PMF | | 0.11 | 0.04 | 0.07 | -0.02 | 0 | 0.43 | 0.89 | 89:0 | 8 | -0.09 |
| Verify score | | -0.63 | -0.13 | -0.53 | 0.12 | 0.13 | 0.08 | 0.44 | 0.56 | 100 | 9. 24 |
| PSI- BLAST | | 3.60E-15 | 1.40E-15 | 1.10E-28 | 7.80E-14 | 9.10E-15 | 5.20E-06 | 5.20E-18 | 1.20E-18 | 2,000 | 3.60E-12 |
| End | | 406 | 554 | 286 | 726 | 749 | 1203 | 1203 | 1203 | | 857 |
| Start AA | | 349 | 498 | 142 | 537 | 995 | 1096 | | 1097 | | 108 |
| Chain | | | | ٧ | ∢ | . ∀ | | ∢ | V | Ţ. | √ |
| PDB DD | | 2adr | 2adr | 2gli | lean | lcun | ldro | 1168 | lfgy | 3 | TPOX |
| SEQ No de | | 756 | 952 | 756 | 757 | 757 | 757 | 757 | 757 | 25 | 79/ |

| | | | | _ | | , | | | | _ |
|------------------|---|---|--|--|---|--|--|---|--|-----------------|
| PDB annotation | MODULE, 2 DIMERIZATION DOMAIN, TRANSFERASE | SIGNAL TRANSDUCTION SAM DOMAIN, EPH RECEPTOR, SIGNAL TRANSDUCTION, OLIGOMER | TYROSINE-PROTEIN KINASE NIAR, RECEPTOR OLIGOMERIZATION, EPH RECEPTORS, TYROSINE 2 PHOSPHORYLATION, SIGNAL TRANSDUCTION, TYROSINE-PROTEIN 3 KINASE | The same of the sa | CACCIUMPHOSPHOLIPID BINDING PROTEIN PIT, CALPACTIN LIGHT CHANN, SIOF FAMILY, EF-HAND PROTEIN, LIGAND OF ANNEKIN II, 2 CALCIUMPHOSPHOLIPID BINDING PROTEIN | CALCIUMPHOSPHOLIPID BINDING PROTEIN PIT, CALPACTIN LIGHT CHANI, SIOW FAMILY, EF-HAND PROTEIN, LIGAND OF ANNEKIN II, 2 CALCIUM/PHOSPHOLIPID BINDING PROTEIN | CALCIUM-BINDING PROTEIN CALMODULIN CERUM TRIC- DOMAIN, RESIDUES 1 - 75, CERUM- LOADED, CALCIUM-BINDING PROTEIN | METAL BINDING PROTEIN S100B, S100BETA; S100BETA; S100BETA; S100BETA; S100BETA; S100B, INRY, DIPOLAK COUPLINGS, EF-HAND, S100 2 PROTEIN, COLCUMA-BINDING PROTEIN, POUR-HELIX BUNDLE, THREE-3 DIMENSIONAL | | |
| Coumpound | A; | EPHB2; CHAIN: A, B, C, D, E, F, G, H; | EPHRIN TYPE-B RECEPTOR 2; CHAIN: NULL; | | SI 00A IO; CHAIN: A, B; | S100A10; CHAIN: A, B; | CALMODULIN; CHAIN: NULL; | S-100 PROTEIN, BETA CHAIN; CHAIN: A, B; | CALCIUM-BINDING PROTEIN CALBINDIN D9K (INTACT FORM) (NMR. 13 STRUCTURES) I CB1 3 | CALCTUM-BINDING |
| SeqFold score | | | | | 69.57 | | | 145.44 | 57.95 | |
| PMF | | -0.02 | -0.02 | | | - | -0.11 | | | 0.99 |
| Verify score | | 0.1 | 0.53 | | | 0.67 | 0.11 | | | 0.43 |
| PSI- BLAST | | 1.10E-14 | 7.20E-14 | | 1.30E-20 | 1.30E-20 | 3.60E-21 | 7.20E-19 | 7.80E-27 | 7.80E-27 |
| End | | 863 | 861 | | 33 | 68 | 18 | 92 | 83 | 82 |
| Start AA | | 793 | 797 | | - | 2 | 4 | | E . | 4 |
| Chain | | ∀ | | | < | ∢ | | ∢ | | |
| PDB DD | | 164f | 18gg | | 184р | 1a4p | lak8 | 1b4c | 1cb1 | <u>19</u> |
| Se o Se | | 762 | 762 | | 763 | 763 | 763 | 763 | 763 | 763 |

| PDB annotation | | | CALCIUM-BINDING PROTEIN CALMODULIN APO TR2C-DOMAIN; ICMF 9 | METAL TRANSPORT CALMODULIN, HIGH RESOLUTION, DISORDER | TRANSPORT PROTEIN CALCIUM BINDING, EF HAND, FOUR-HELIX BUNDLE | CALCIUM-BNDING CALCIUM- BNDING, ZINC, METAL-BNDING, ACETYLATION | | CALCIUM-BINDING PROTEIN CALCIUM-BINDING PROTEIN, CALCIUM-DEPENDENT PROTEASE, APO 2 FORM, SMALL, SUBUNIT | STRUCTURAL PROTEIN HELIX-TURN- HELIX | METAL TRANSPORT CALMODULIN, HIGH RESOLUTION, DISORDER | METAL BINDING PROTEIN YEAST FREQUENIN EF-HAND, CALCIUM | CALCIUM-REGULATED MUSCLE | CONTRACTION MUSCLE CONTRACTION, CALCIUM-BINDING, | TROPONIN, E-F HAND, 2 OPEN CONFORMATION REGULATORY | DOMAIN, CALCIUM-REGULATED 3 |
|------------------|--|--|---|--|---|---|---|--|---|--|---|--------------------------|--|---|-----------------------------|
| Coumpound | PROTEIN CALBINDIN D9K (INTACT FORM) (NMR, 13 STRUCTURES) 1CB13 | CALCIUM-BINDING PROTEIN CALMODULIN COMPLEXED WITH CALMODULIN-BINDING DOMAIN OF 10DM 3 CALMODULIN-EPERDENT FROTEIN KINASE II 10DM 4 | CALMODULIN (VERTEBRATE); ICMF 6 CAI CHAIN: NULL; ICMF 7 ICM | .¥: | CALMODULIN; CHAIN: A; TRA BIN BUN | S-100 PROTEIN; CHAIN: CAI | CONTRACTILE SYSTEM PROTEIN TROPONIN C 1 TOP 3 | CALPAIN; CHAIN: A, B; CAI CAI CAI | TROPONIN C; | JLIN; CHAIN: A; | CALCIUM-BINDING ME PROTEIN NCS-1; CHAIN: A; FRE | ٠, | 38 | SE 50 | DOI |
| SeqFold score | PROT (INTA STRU | CALC PROT COMF CALM DOM CALM CALM | CALIN (VER) CHAI | CALIN | CALN | 137.02 S-100 NULL | CONT PROT 3 | CALP | CARDIAC CHAIN: A; | CALI | CALC | TROP | | | |
| PMF | | 0.06 | 0.15 | -0.17 | 81.0 | | -0.07 | 0.09 | 0.28 | 0.39 | -0.03 | 0.47 | | | |
| Verify | | 0.21 | 0.17 | 90:00 | -0.17 | | 0.07 | -0.18 | -0.29 | -0.18 | 0.05 | -0.12 | | | |
| PSI- BLAST | | 9.00E-21 | 7.20E-21 | 3.60E-23 | 7.20E-20 | 1.40E-16 | 7.20E-20 | 2.60E-09 | 2.60E-09 | 1.30E-09 | 2.60E-08 | 3.90E-10 | | | |
| End | | 81 | 81 | . 68 | 18 | 68 | 92 | 252 | 252 | 252 | 252 | 252 | | | |
| Start AA | | 4 | _ | 4 | | 2 | \$ | 135 | 131 | 129 | 129 | 135 | | | |
| Chain D | | Y | | ٧ | ¥ | | | A | Ą | ¥ | ٧ | | | | |
| PDB ID | | Icd m | lcmf | lexr | 1121 | 1mh 0 | 1top | 1aj5 | ₽ | lexr | Ifpw | Itcf | | | |
| SEQ No. | | 763 | 763 | 763 | 763 | 763 | 763 | 766 | 766 | 992 | 992 | 992 | | | |

| | _ | | | | _ | | , | _ | | | | | _ |
|----------------|----------------------|---|---|--|----|---|--|---|--|--|--|--|----------------------|
| PDB annotation | MUSCLE CONTRACTION . | CALCIUM-BINDING PROTEIN EF- HAND ITNX 14 | | | | MEMBRANE PROTEIN AQPI WATER PARNNEL, TWO-DIMENSIONAL CRYSTAL, ELECTRON 2 DIFFRACTION, ELECTRON MICROSCOPY | MEMBRANE PROTEIN AQPI WATER PANNEL, TWO-DIMENSIONAL CRYSTAL, ELECTRON 2 DIFFRACTION, ELECTRON MICROSCOPY | | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGNIN, C2-DOMAIN, EXOCYTOSIS, NEUROTRANSMITTER 2 RELEAS, ENDOCYTOSIS/EXOCYTOSIS | ENDOCYTOSIS/EXOCYTOSIS NSECI; PROTEIN-PROTEIN COMPLEX, MULTI-SUBUNIT | ENDOCYTOSIS/EXOCYTOSIS BETA SANDWICH, CALCIUM ION, C2 DOMAIN | TRANSFERASE CALCIUM++, PHOSPHOLIPID BINDING PROTEIN, CACCIUM-BINDING 2 PROTEIN, PHOSPHATIDYLSERINE, PROTEIN YNASSE | |
| Coumpound | | TROPONIN C; ITNX 4 CHAIN: NULL; ITNX 5 | CALCIUM BINDING PROTEIN CALMODULIN (TRE-CS PRAGMENT COMPAISING RESIDUES 78- 148 ITRC 3 OF THE INTACT MOLECULE) 1TRC 4 | CALCTUM-BINDING PROTEIN PARVALBUMIN (ALPHA LINEAGE) 5PAL 3 | | AQUAPORIN-1; CHAIN: A; | AQUAPORIN-1; CHAIN: A; | | SYNAPTOTAGMIN I; CHAIN: A; | SYNTAXIN BINDING PROTEIN 1; CHAIN: A; SYNTAXIN 1A; CHAIN: B; | SYNAPTOTAGMIN III; CHAIN: A; | PROTEIN KINASE C, ALPHA TYPE; CHAIN: A; | CALCIUM/PHOSPHOLIPID |
| SeqFold | | | | | | | | | | | | | |
| PMF | | 16.0 | 0.95 | 0.53 | | 0.51 | 0.88 | | 0.94 | 0.01 | 0.82 | 0.71 | _ |
| Verify | | -0.53 | -0.37 | 0.27 | | -0.22 | -0.13 | | 0.21 | -0.13 | 0.38 | 0.48 | 0.3 |
| PSI- BLAST | | 1.00E-10 | 1.30E-08 | 1.30E-08 | | 1.106-73 | 3.90E-76 | | 1.30E-11 | 5.20E-05 | 6.50E-07 | 0.0026 | 6.50E-12 |
| End | | 252 | 252 | 252 | | 227 | 227 | | 664 | 252 | 647 | 999 | 664 |
| Start | | 140 | 194 | 171 | | | 6 | | 541 | 26 | 541 | 541 | 541 |
| Chain | | | ¥ | | | ¥ . | ∢ | | ¥ | В | Ą | ¥ | |
| EQB CD | | Itrx | 로 | Spal | | 1fgy | Ifqy | | 1byn | 1dh1 | ldqv | Idsy | lısy |
| SEQ B B Ö | | 992 | 766 | 766 | -+ | | 768 | | | 769 | 692 | 694 | 992 |

| | | _ | | | | | | | | | | |
|----------------|---|---|--|--|--|--|--|---|---|---|---|---|
| PDB annotation | | , | P21; SOS; COMPLEX (ONCOGENE PROTEIN/EXCHANGE FACTOR), SMALL GTPASE, 2 EXCHANGE FACTOR | P21; SOS; COMPLEX (ONCOGENE PROTEIN/EXCHANGE FACTOR), SMALL GTPASE, 2 EXCHANGE FACTOR | P2I; SOS; COMPLEX (ONCOGENE PROTEIN/EXCHANGE FACTOR), SMALL GTPASE, 2 EXCHANGE FACTOR | SIGNAL TRANSDUCTION PROTEIN | CYTOSKELETON | | SIGNALING PROTEIN DAPPI, PHISH, BAM32; PLEKSKTRIN, 3-PHOSPHOINOSITIDES, INOSITOL TETRAKISPHOSPHATE 2 SIGNAL TRANSDUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN DAPPI, PHISH, BAM32; PLECKSTRIN, 3. PHOSPHOINOSITIDES, INOSITIDE, TETRAKISPHOSPHATE 2 SIGNAL TRANSDUCTION PROTEIN, ADAPTOR PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN ARFI GUANINE NUCLEOTIDE EXCHANGE FACTOR AND PH DOMAIN | |
| Соитроипд | BINDING PROTEIN SYNAPTOTAGMIN I (FIRST C2 DOMAIN) (CALB) IRSY 3 | | H-RAS, CHAIN: R; SON OF SEVENLESS-1; CHAIN: S; | H-RAS; CHAIN: R; SON OF SEVENLESS-1; CHAIN: S; | H-RAS, CHAIN: R; SON OF SEVENLESS-1; CHAIN: S; | BETA-SPECTRIN; 1BTN 4 CHAIN: NULL; 1BTN 5 | BETA-SPECTRIN; IDRO 6 CHAIN: NULL; IDRO 7 | SIGNAL TRANSDUCTION PROTEIN DYNAMIN (PLECKSTRIN HOMOLOGY DOMAIN) (DYNPH) 1DYN 3 | DUAL ADÁPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | DUAL ADAPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | GRP1; CHAIN: A; | PHOSPHORYLATION PLECKSTRIN (N-TERMINAL |
| SeqFold | | | 79.72 | | | | | | | | | |
| PMF | | | | _ | _ | 89.0 | 9.4 | 0.25 | | 0.05 | 0.36 | 0.24 |
| Verify | | | | 0.2 | 0.26 | -0.09 | -0.22 | -0.04 | 0.3 | 0.04 | 0.35 | -0.02 |
| PSI- BLAST | | | 9.10E-77 | 9.10E-77 | 7.20E-61 | 1.40E-18 | 7.20E-12 | 5.40E-06 | 1.00E-07 | 1.30E-12 | 1.10E-16 | 1.10E-13 |
| End AA | | | 311 | 291 | 312 | 541 | 246 | 241 | 546 | 539 | 546 | 542 |
| Start | | | | 13 | 41 | 438 | 439 | 456 | 429 | 441 | 447 | 437 |
| Chain | | | S | S | s | | | < | ∢ | ∢ | ¥ | |
| 203 El | | | 1bkd | 1 pkd | 1bkd | 1btn | 1dro | ldyn | 1168 | 1168 | Ifgy | 1pls |
| SEQ NO. | | | 0,1 | 770 | 0/1 | 170 | 770 | 770 | 770 | 0/1 | 770 | 170 |

| | | | | | _ | | | | _ | | | | | | _ | | | _ | _ | | | |
|------------------|--|---|---|----------------------------------|-----------------------|--------------------------------|--|--------------------------------|-----------------------|--|--------------------------------|-----------------------|--------------------------------|---|--------------------------------|-----------------------|--------------------------------|----------------------------|---|---|--------------------------------|--|
| PDB annotation | | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (7 INC PINGER/INA) 7 INC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER, DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/UNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) |
| Coumpound | PLECKSTRIN HOMOLOGY DOMAND, MITANT I PLS.3 WITH LEU GLU (HIS)6 ADDED TO THE C LERMINUS I PLS.4 (INS/G105- LEHHHHHH) (NMR, 25 STRUCTURES) I PLS.5 | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE, CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | DNA: CHAIN: A B D F: | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | DNA: CHAIN: A, B, D. E, | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C. F, G; | | 2 4 4 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | |
| SeqFold score | | | 78.23 | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.99 | | - | | | | 1 | | | - | | | | - | | | | | _ | | |
| Verify | | 0.19 | | 0.37 | | | | 0.29 | | | 0.46 | | | | 0.29 | | | | 35.0 | 5 | | |
| PSI- BLAST | | 6.50E-41 | 5.20E-45 | 5.40E-46 | ! | | | 3.60E-47 | | | 1.80E-48 | | | | 1.10E-49 | | | | 2 505 51 | 3.002-31 | | |
| End | | 210 | 351 | 209 | | | | 237 | | | 265 | | | | 293 | | | | 277 | //ς | | |
| Start AA | | 181 | 269 | 128 | | | | 156 | | | 184 | | | | 212 | | | | 300 | 067 | | |
| Chain ID | | ٧ | ۷ | ပ | | | | ၁ | | | ၁ | | | | J | | | | c | ر | | |
| PDB ID | | lalh | lalh | Ime | > | | | Іше | ^ | | 1me | ۲, | | | 1me | ^ | | | Tme |) × | | |
| SEQ D NO: | · | 772 | 27. | 772 | | | | 772 | | | 7.1.1 | | | | 772 | | | | 777 | 711 | | |

| PDB annotation | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC PRINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL, STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGH, 2 CRYSTAL, STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (TRANSCRIPTION REGULATIONIDNA) COMPLEX (TRANSCRIPTION REGULATIONIDNA), RNA REGULATIONIDNA), RNA POLYMERAE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER REOTEIN | COMPLEX (TRANSCRIPTION REGULATIONIDNA) COMPLEX (TRANSCRIPTION REGULATIONIDNA), RNA REGULATIONIDNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER REOTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA |
|------------------|--|---|---|--|---|--|---|--|
| Coumpound | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA, CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA, CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA, CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; |
| SeqFold score | 102.88 | | | | | 115.72 | | |
| PMF | | | _ | 1 | 0.42 | | 0.76 | 0.94 |
| Verify | | 0.16 | 0.33 | 0.44 | 90.0d | | 0.22 | 60.0 |
| PSI- BLAST | 3.60E-51 | 3.60E-51 | 7.20E-51 | 7.205-51 | 5.40E-43 | 5.20E-73 | J.10E-36 | 1.30E-37 |
| End | 378 | 405 | 433 | 461 | 181 | 298 | 274 | 443 |
| Start | 296 | 324 | 352 | 380 | . 66 | 126 | 129 | 297 |
| Chain ID | ပ | ပ | ၁ | ပ | ပ | V | ∢ | 4 |
| FDB OI | J. J. J. J. J. J. J. J. J. J. J. J. J. J | y Ime | Ime y | Ime y | Jme y | 146 | \$ <u>1</u> | 1116 |
| ğa ÿ | 772 | 772 | 772 | 2772 | 277 | 772 | 772 | 772 |

| | | | | | | | | | | | | _ | | | | | _ | | | | | | | | _ | | |
|-----------------|---|--|--|--|--|---|------------------------|--|--------------------------------|-----------------------------|---|------------------------|------------------------------|------------------------------|-----------------------------|------------------------|------------------------|------------------------------|---------------------------|--------------------------------|-----------------------------|------------------------|------------------------|------------------------------|---------------------------|---|------------------------|
| PDB annotation | POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX TO ANSCRIPTION | (TRANSCRIFTION) REGULATION/DIA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX | (TRANSCRIPTION REGULATION/DNA), RNA | POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGIL ATTONIONA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG I; | INTIATOR ELEMENT, YYL ZING 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG I; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YYI, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN DNA PROTEIN | RECOGNITION, 3 COMPLEX |
| Coumpound | | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, E. | CITAIN. B, C, E, F, | TFIIIA; CHAIN: A, D; SS RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | | YYI; CHAIN: C; ADENO- | ASSOCIATED VIRUS PS INITIATOR FI.EMENT DNA: | CHAIN: A, B; | | | YYI; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | CHAIN: A. B. | | | VVI CHAIN C. ADENO. | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | YYI: CHAIN: C. ADENO- | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | |
| SeqFold | | | | | | - | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 96.0 | | 0.15 | | | 0.87 | | | | | 1 | | | | | _ | | | | | | _ | | | | |
| Verify score | | 0.15 | | -0.27 | | | 0.12 | | | | | 0.32 | | | | | 0.2 | | | | | | 0.3 | | | | |
| PSI- BLAST | | 1.80E-36 | | 3.60E-33 | | | 3.90E-42 | | | | | 1.80E-32 | | | | | 6.50E-52 | | | | | | 1.30E-53 | | | | |
| End | | 461 | | 218 | | | 509 | | | | | 237 | | | | | 237 | | | | | | 266 | | | | |
| Start AA | | 325 | | 72 | | | 120 | | | | | 131 | | | | | 133 | | | | | | 154 | | | | |
| Chain D | | ¥ | | ٧ | | | ပ | | _ | | | ပ | | | | | C | | | | | | U | | | | |
| PDB DD | | 1466 | | 9,410 | | | Inbd | | | | | Iubd | | | | | Iubd | | _ | | | | Pg. | | | | |
| SEQ No: | | 772 | | 772 | | | 772 | | | | | 772 | | | | | 772 | | _ | | | | 772 | | | | |

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|----------------|--------------------------------|---|---|---|------------------------|------------------------------|-------------------------------|-----------------------------|--|------------------------|------------------------------|---------------------------|---|-----------------------|--------------------------------|------------------------|------------------------------|---------------------------|--------------------------------|----------------------|--------------------------------|------------------------|------------------------------|---------------------------|----------------------------|-----------------------|--------------------------------|------------------------|------------------------------|-------------------------------|-----------------------------|
| PDB annotation | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGILLATION (DAY) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | INTIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YYL, ZINCZ FINGER PROTEIN DNA-PROTFIN | RECOGNITION 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YYI, ZINC 2 | PECCENTION 2 COMPLEY | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG I; | TRANSCRIPTION INITIATION, | ENICED BEOTER! DAY PROTEIN | RECOGNITION 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | INTIATOR ELEMENT, YYI, 2INC 2 | FINGER PROTEIN, DNA-PROTEIN |
| Coumpound | | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; | CHAIN: A, B; | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS PS | CHAIN: A, B; | | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | YYI; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | CHARL A B. | Chain: A, B; | | | YYI; CHAIN: C; ADENO- | ASSOCIATED VIRUS PS | CHAIN: A, B; | |
| SeqFold | | 89.18 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | | | | 0.92 | | | | | 96.0 | | | | | | 86.0 | | | | | | 1 | | | | | | 0.95 | | | |
| Verify | | | | | -0.04 | | | | | 0.26 | | | | | | 0.22 | | | | | | 91.0 | | | | | | 9.4 | | | |
| PSI- BLAST | | 7.80E-55 | | | 7.80E-55 | | | | | 6.50E-56 | | | | | | 1.60E-35 | | | | 1 | | 1.30E-56 | | | | | | 5.20E-51 | | | |
| End | | 322 | | | 349 | | | | | 405 | | | | | | 405 | | | | | | 434 | | | | | | 461 | | | |
| Start AA | | 212 | | | 238 | | | | | 294 | | | | | | 304 | | | | | | 322 | | | | | | 350 | | | |
| Chain D D | | ပ | | | ပ | | | | | Ç | | | | | | ပ | | | | | | ၁ | | | | | | ၁ | | | |
| EQ EI | | 1ubd | | | Iubd | | | | | lubd | | | | | | 1npq | | | | | | Inbd | | | | | | pqn1 | | | |
| S e S | | 21.1 | | | 772 | | | | | 772 | | | | | | 712 | | | | | | 71 | | | | | | 7.1.2 | | | |

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|----------------|---|--|--------------------------------|-----------------------------|--|---------------------------|---------------------------------|----------------------|---------------------------|------------------------------------|--|---------------------------|------------------------------------|----------------------------|----------------------|---------------------------|-----------------------------|----------------------|---------------------------|------------------------------------|--|---------------------------|------------------------------------|----------------------------|---------------------------|------------------------------------|----------------------------|----------------------|---|--|
| PDB annotation | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG I; TO ANSCRIPTION INITIA TION | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (DNA-BINDING | ZINC FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | SINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | ZINC FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | ZINC FINGER COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | ZINC FINGER, COMPLEX (DNA- | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI, GLI, | ZINC FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN DNA SIVE ENCER CT I. CT | ZINC FINGER, COMPLEX (DNA-BINDING PROTEIN/DNA) |
| Coumpound | | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 NITT A TOB ET EMENT DAIA. | CHAIN: A, B; | | | ZINC FINGER PROTEIN GLII; | CHAIN: A; DINA; CHAIN: C, D; | | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, | ń | ZINC FINGER PROTEIN GLI1; | CHAIN: A; DNA; CHAIN: C, | á | | ZINC FINGER PROTEIN GLII: | Challe. A, Diva, Challe. C. | S. | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, | ÷. | ZINC FINGER PROTEIN GLI1; | CHAIN: A; DNA; CHAIN: C, | Ċ | ZINC FINGER PROTEIN GLIT: | CHAIN: A; DNA; CHAIN: C, | Ď, | | ZINC FINGER PROTEIN GLII; | D; |
| SeqFold | | | | | | | | | | | | | | | | 98.73 | | | | | | | | | Ī | | | | | |
| PMF | | 0.92 | | | | 0.88 | | | _ | | | 92.0 | | | | | | | 6.03 | | | 0.84 | | | 96.0 | | | | | |
| Verify | | 0.32 | | | | 0.21 | | | 0.35 | | | 91.0 | | | | | | | 9.4 | | | 0.24 | | | 0.35 | | | | 0.47 | |
| PSI- BLAST | | 1.80E-34 | | | | 2.60E-54 | | | 3.60E-33 | | | 3.90E-66 | | | | 1.00E-71 | | | 1.00E-71 | | | 7.20E-33 | | | 6.50E-67 | | | 1000 | 5.40E-34 | |
| End AA | | 461 | | | | 239 | | | 264 | | | 295 | | | | 351 | | | 407 | | | 432 | | | 461 | | | ļ | 94 | |
| Start | | 360 | | | | 121 | | | 128 | | | 128 | | | | 212 | | | 268 | | | 304 | | | 324 | | | | 725 | |
| Chain | | ပ | | | | V | | | ∢ | | | A | | | | < | | | V | | | ¥ | | | 4 | | | | ∢ | |
| PDB CI | | lubd | | | | 2gli | | | 2gli | | | 2gli | | | | 7gli | | | 2gli | | | 2gli | | | 2gli | | | | 187 | |
| SEQ El S | | 712 | | | | 772 | | | 21.2 | | | 772 | | | 1 | 7// | | | 712 | | | 21. | | | 772 | | | 1 | 7 | |

| PDB annotation | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | HYDROLASE TETRATRICOPEPTIDE, TRP, HYDROLASE, PHOSPHATASE, PROTEIN-PROTEIN INTERACTIONS, TPR, 2 SURER-HELIX, X-RAY | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELICAL REPEAT, HSP90, 2 PROTEIN BINDING | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELICAL REPEAT, HSC70, 2 HSP70, PROTEIN BINDING | SIGNALING PROTEIN PEROXISMORE RECEPTOR 1, PTS1-BP. PEROXIN-5, PTS1 PROTEIN-PEPTIDE COMPLEX, TETRATRICOPEPTIDE REPEAT, TPR, 2 HELICAL REPEAT | AMIDOTRANSFERASE AMIDOTRANSFERASE, THIOESTER | AMIDOTRANSFERASE AMIDOTRANSFERASE, THIOESTER | LYASE AIRC, PURK; ATP-GRASP, CARBOXYPHOSPHATE, PURINE BIOSYNTHESIS, LYASE | LIGASE ATP-GRASP, CARBOXYLASE, BIOTIN-DEPENDENT | LIGASE LMDDL2; ATP-BINDING. GRASP MOTIF FOR ATP. |
|-----------------|--|--|--|--|---|---|--|--|---|--|---|
| Coumpound | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | SERINDTHREONINE PROTEIN PHOSPHATASE 5; CHAIN: NULL; | TPR2A-DOMAIN OF HOP; CHAIN: A; HSP90-PEPTIDE MEEVD; CHAIN: B; | TPR1-DOMAIN OF HOP; CHAIN: A, B; HSC70- PEPTIDE; CHAIN: C, D; | PEROXISOMAL TARGETING SIGNAL I RECEPTOR; CHAIN: A, B; PTSI- CONTAINING PEPTIDE; CHAIN: C, D; | CARBAMOYL PHOSPHATE SYNTHETASE; CHAIN: A, B, C, D, E, F, G, H; | CARBAMOYL PHOSPHATE SYNTHETASE; CHAIN: A, B, C, D, E, F, G, H; | N5- CARBOXYAMINOIMIDAZOL E RIBONUCLEOTIDE CHAIN: A: | BIOTIN CARBOXYLASE; CHAIN: A. B. | D-ALANINE:D-LACTATE LIGASE; CHAIN: A, B; |
| SeqFold | | | | | | | | | | | |
| PMF score | -0.05 | 0.15 | 0.77 | 89.0 | 0.74 | 0.99 | 6:0 | 96:0 | -0.11 | 0.54 | 0.45 |
| Verify score | 0.07 | -0.01 | 0.09 | 0.14 | 0.12 | 0.47 | 0.14 | 0.49 | 0.07 | 0.32 | 0.07 |
| PSI- BLAST | 9.00E-28 | 5.40E-31 | 1.30E-08 | 9.10E-08 | 6.50E-10 | 6.50E-09 | 1.80E-64 | 1.10E-39 | 1.80E-16 | 1.30E-86 | 9.00E-37 |
| End | 081 | 211 | 180 | 180 | 180 | 179 | 098 | 892 | 828 | 965 | 858 |
| Start AA | 90 | 7.1 | 105 | 105 | 105 | 105 | 454 | 529 | 532 | 534 | 531 |
| Chain ID | A | A | | ¥ | ¥ | Ą | Ą | Ą | ¥ | Ą | V |
| PDB ID | 2gli | 2gli | la17 | le! | lelw | 1fch | 1a9x | 1a9x | 1b6r | ldvl | lehi |
| SEQ NO: | 111 | 772 | 773 | 773 | 773 | 773 | 774 | 774 | 774 | 774 | 774 |

| PDB annotation | LIGASE LMDDL2; ATP-BINDING. GRASP MOTIF FOR ATP. | LIGASE, GTP-SPECIFIC LIGASE, GTP-SPECIFIC | TRANSFERASE TRANSFORMYLASE, PURINE BIOSYNTHESIS, ATP-GRASP | TRANSFERASE TRANSFORMYLASE, PURINE BIOSYNTHESIS, ATP-GRASP | LIGASE PURD GEN PRODUCT, GAR- SYN, GLYCINAMIDE RIBONUCLEOTIDE SYNTHETASE, ATP-GRASP, 2 PURINE DE NOVO BIOSYNTHETIO PATHWAY, | LIGASE DD-LIGASE, DDLB; GLYCOGEN PHOSPHORYLASE, LIGASE, CELL WALL, PEPTIDOGLYCAN 2 SYNTHESIS, VANCOMYCIN, ADP BINDING | LIGASE SCS; SCS; CITRIC ACID CYCLE, HETEROTETRAMER, LIGASE | TRANSLATION PROTEIN-PROTEIN COMPLEX | INTEGRIN INTEGRIN, CELL ADHESION, GLYCOPROTEIN | INTEGRIN INTEGRIN, CELL ADHESION, GLYCOPROTEIN | NTEGRIN NTEGRIN, CELL |
|------------------|---|--|---|---|---|---|--|---|--|--|------------------------|
| Coumpound | D-ALANINE:D-LACTATE LIGASE; CHAIN: A, B; | SUCCINYL-COA SYNTHEITASE, ALPHA CHAIN; CHAIN: A; SUCCINYL-COA SYNTHEITASE, BETA CHAIN; CHAIN: B; | PHOSPHORIBOSYLGLYCINA MIDE FORMYLTRANSFERASE 2; CHAIN: A, B; | PHOSPHORIBOSYLGLYCINA MIDE FORMYLTRANSFERASE 2; CHAIN: A, B: | GLYCINAMIDE RIBONUCLEOTIDE SYNTHETASE, CHAIN: A; | D-ALAND-ALA LIGASE; CHAIN: NULL; | SUCCINYL-COA LIGASE; CHAIN: A, D; SUCCINYL- COA LIGASE; CHAIN: B, E; | ELONGATION FACTOR EEFIA, CHAIN: A; ELONGATION FACTOR EEFIBA; CHAIN: B; | INTEGRIN ALPHA 2 BETA; CHAN: A. B: | NTEGRIN ALPHA 2 BETA; CHAIN: A, B; | INTEGRIN ALPHA 2 BETA; |
| SeqFold score | | | | | | | | | | 84.82 | |
| PMF | 0.63 | 0.07 | 0.99 | 0.11 | 0.37 | 0.18 | 0.07 | _ | _ | | |
| Verify score | 0.22 | -0.04 | 0.51 | 0.21 | 0.2 | -0.07 | 0.04 | 1.05 | 99.0 | | 0.74 |
| PSI- BLAST | 1.80E-36 | 7.20E-22 | 6.50E-30 | 1.40E-39 | 3.60E-54 | 1.80E-43 | 1.80E-27 | 0 | 9.00E-28 | 9.00E-28 | 7.20E-28 |
| End | 828 | 854 | 953 | 098 | 868 | 829 | 844 | 443 | 313 | 316 | 204 |
| Start AA | 531 | 929 | 533 | 534 | 531 | 530 | 929 | 2 | 611 | 120 | 321 |
| Chain | В | m | V | ٧ | ∢ | | eq. | V | A | V : | A |
| 8 a | 를 - | leuc | leyz | leyz | Igso | liow | 2scu | 1160 | laox | laox | laox |
| Š e Š | 774 | 774 | | 774 | 41.4 | 774 | 774 | 277 | 9/1 | 776 | 776 |

| | _ | | | | | | | | | | | | | | | | | | _ | | | | | | | | | |
|----------------|------------------------|--|--|---------------------------|--|------------------------------|--|------------------------------|------------------------|------------------------------|------------------------|-----------------|---|------------------------------|--------------------------------------|------------------------------|--------------------------|------------------------------|------------------------------|-----------------------------|--|-------------------------|------------------------------|-----------------------------|-----------------------------|------------------------|--------------------------------|--|
| PDB annotation | ADHESION, GLYCOPROTEIN | COLLAGEN-BINDING COLLAGEN- BINDING, HEMOSTASIS, | COLLAGEN-BINDING COLLAGEN- BINDING, HEMOSTASIS, | DINUCLEOTIDE BINDING FOLD | COLLAGEN-BINDING COLLAGEN- BINDING, HEMOSTASIS, DINUCLECITIDE BINDING FOLD | WILLEBRAND WILLEBRAND, BLOOD | COAGULATION, PLATELET, GLYCOPROTEIN | WILLEBRAND WILLEBRAND, BLOOD | COAGULATION, PLATELET, | WILLEBRAND WILLEBRAND, BLOOD | COAGULATION, PLATELET, | GLTCOFROIEIN | STRUCTURAL PROTEIN FDOMAIN, METAL BINDING, COLLAGEN, ADHESION | STRUCTURAL PROTEIN I-DOMAIN, | METAL BINDING, COLLAGEN, ADHESION | IMMUNE SYSTEM VON WILLEBRAND | FACTOR, GLYCOPROTEIN IBA | (A:ALPHA) BINDING, 2 COMPLEX | (WILLEBRAND/IMMUNOGLOBULIN), | BLOOD COAGULATION TYPE 3 2B | VON WILLEBRAND DISEASE NAME EVETEM VON UR! 1 EPR AND | EACTOR OF VOORDOTERNIES | (A:AI.PHA) BINDING 2 COMPLEX | CWILLEBRAND/IMMUNOGLOBILIN) | BLOOD COAGULATION TYPE 3 2B | VON WILLEBRAND DISEASE | CELL ADHESION PROTEIN A-DOMAIN | INTEGRIN, CELL ADHESION PROTEIN, GLYCOPROTEIN, EXTRACELLII AR 2 MATRIX |
| Coumpound | CHAIN: A, B; | VON WILLEBRAND FACTOR; CHAIN: A, B; | VON WILLEBRAND FACTOR; CHAIN: A, B; | | VON WILLEBRAND FACTOR; CHAIN: A, B; | A1 DOMAIN OF YON | WILLEBRAND FACTOR; CHAIN: NULL: | AI DOMAIN OF VON | WILLEBRAND FACTOR; | AI DOMAIN OF VON | WILLEBRAND FACTOR; | DEFECTIVE NOLL; | IN EGKUN ALPHA-I; CHAIN: A, B; | INTEGRIN ALPHA-1; CHAIN: | A, B; | IMMUNOGLOBULIN NMC-4 | IGGI; CHAIN: L; | IMMUNOGLOBULIN NMC-4 | IGGI; CHAIN: H; VON | WILLEBRAND FACTOR; | CHAIN: A; | IGGI: CHAIN: 1 | IMMINOGLOBILIN NMC-4 | IGGI: CHAIN: H: VON | WILLEBRAND FACTOR: | CHAIN: A; | INTEGRIN; CHAIN: NULL; | |
| SeqFold | | | 94.53 | | | | | 86.49 | | | | | | | | | | | | | | | | | | | | |
| PMF score. | | _ | | | - | 69.0 | | | | _ | | 1 | _ | _ | | 0.75 | | | | | - | | | | | | _ | |
| Verify | | 9.76 | | | 99.0 | 0.42 | | | 1 | 0.78 | | 9,0 | 6:0 | 0.85 | | 0.27 | | | | | 780 | 5 | | | | | 0.7 | |
| PSI- BLAST | | 9.00E-24 | 9.00E-24 | | 1.80E-21 | 3.60E-32 | | 7.20E-29 | | 7.20E-29 | | 1 905 70 | 1.60E-28 | 3.60E-30 | | 7.20E-31 | | | | | 3 60F-78 | 2000 | | | | | 2.60E-30 | |
| End | | 293 | 305 | | 492 | 317 | | 509 | | 208 | | 300 | S S | 200 | | 314 | | | | | 507 | 3 | | | | | 267 | |
| Start AA | | 721 | 122 | | 324 | 110 | | 311 | | 313 | | 133 | 3 | 324 | | 119 | | | | | 310 | ; | | | | | 124 | |
| Chain | | A | A | | < | | | | | | | - | £ | Ą | | ٧ | | | | | \ \ | | | | | | | |
| 708 U | | latz | latz | | latz | lauq | | lauq | | land | | Polo | ± | 1ck4 | | 1fms | | | | | File |] | | | | | lido | |
| S B S | | 91.1 | 9/1 | | 9/1 | 9// | - | 216 | | 276 | | 77.6 | 2 | 176 | | 776 | | | | | 176 | : | | | | | 92 | |

| PDB annotation | CYTOSKELETON | CELL ADHESION PROTEIN A-DOMAIN INTEGRIN, CELL ADHESION | PROTEIN, GLYCOPROTEIN, EXTRACELLULAR 2 MATRIX, | CYTOSKELETON | INTEGRIN, CELL ADHESION | PROTEIN, GLYCOPROTEIN, | EXTRACELLULAR 2 MATRIX, CYTOSKELETON | CELL ADHESION PROTEIN A-DOMAIN | INTEGRIN, CELL ADHESION | PROTEIN, GLYCOPROTEIN, | EXTRACELLULAR 2 MATRIX, | CELL ADHESION PROTEIN A-DOMAIN | INTEGRIN, CELL ADHESION | PROTEIN, GLYCOPROTEIN, | EXTRACELLULAR 2 MATRIX, | CYTOSKELETON | CELL ADHESION LFA-1, ALPHA- | LUBETA-2 INTEGRIN, A-DOMAIN; ILFA 8 | CELL ADHESION LFA-1, ALPHA- | L\BETA-2 INTEGRIN, A-DOMAIN; ILFA 8 | CELL ADHESION LFA-1, ALPHA- | L'BETA-2 INTEGRIN, A-DOMAIN; ILFA 8 | CELL ADHESION INTEGRIN, CELL | ADHESION | | CELL ADHESION INTEGRIN, CELL | ADHESION | | SCAFFOLD PROTEIN SCAFFOLD PROTEIN, PP2A, PHOSPHORYLATION, | HEAT REPEAT | TRANSPORT PROTEIN SERINE-RICH |
|-----------------|--------------|--|---|-----------------------|----------------------------|------------------------|---|--------------------------------|-------------------------|------------------------|-------------------------|--------------------------------|-------------------------|------------------------|-------------------------|--------------|-----------------------------|--|-----------------------------|--|-----------------------------|--|------------------------------|------------------------|---------------------|------------------------------|------------------------|---------------------|---|-------------|-------------------------------|
| Coumpound | | INTEGRIN; CHAIN: NULL; | | Purposed Ottable Sure | IN I ECKLIN, CHAIN: INOLL, | | | INTEGRIN; CHAIN: NULL; | | | | INTEGRIN; CHAIN: NULL; | | | | | CDIIA; ILFA 5 CHAIN: A, B; | LFA 6 | CDI IA; ILFA 5 CHAIN: A, B; | ILFA 6 | CDI1A; 1LFA 5 CHAIN: A, B; | ILFA 6 | ALPHAI BETAI INTEGRIN; | CHAIN: A; ALPHAI BETAI | INTEGRIN; CHAIN: B; | ALPHAI BETAI INTEGRIN; | CHAIN: A; ALPHAI BETAI | INTEGRIN; CHAIN: B; | PROTEIN PHOSPHATASE PP2A; CHAIN: A, B; | | KARYOPHERIN ALPHA; |
| SeqFold | | | | 12.00 | 1/.96 | | | | | | | | | | | | | | 90.24 | | | | | | | | | | | | |
| PMF score | | _ | | | | | | - | | | | _ | | | | | _ | | | | _ | | _ | | | _ | | | 0.17 | | _ |
| Verify score | | 0.62 | | | | | | 0.57 | | | | 0.54 | | | | | 0.42 | | | | 0.85 | | 0.7 | | | 69:1 | | | 0.02 | | 0.52 |
| PSI- BLAST | | 5.40E-27 | | 0 100 44 | 3.105-44 | | | 9.10E-44 | | | | 9.00E-26 | | | | | 3.60E-23 | | 3.60E-24 | | 3.60E-24 | | 7.20E-28 | | | 1.60E-29 | | | 3.60E-33 | 4, 200 | 3.60E-49 |
| End | | 307 | | 400 | ş | | | 497 | | | | 498 | _ | | | | 268 | | 201 | | 503 | | 309 | | | 499 | | | 343 | 1 | 275 |
| Start AA | | 124 | | 200 | 120 | | | 325 | | | | 326 | | | | | 123 | | 323 | | 326 | | 122 | | | 324 | | | | | |
| Chain ID | | | | | | | | | | | | | | _ | | | ∢ | | V | | ¥ | | V | | | ¥ | | | ∢ | | A |
| PDB ID | | lido | | 13.5 | 2 | | | - Sil | | | | lido | | | | | Ilfa | | -II | | 뢜 | | lqc5 | | 1 | 1965 | | Ī | 163u | | 58 |
| SEQ NO: | | 776 | | 766 | ? | | | 27.6 | | _ | | 776 | | | | | 9/ | | 176 | | 9// | | 276 | | | 176 | | I | 111 | | |

| PDB annotation | RNA POLYMERASE I SUPPRESSOR PROTEIN; ARM REPEAT | TRANSPORT PROTEIN SERINE-RICH RNA POLYMERASE I SUPPRESSOR PROTEIN; ARM REPEAT | NUCLEAR IMPORT RECEPTOR KARYOPHERIN ALPHA, NUCLEAR IMPORT RECEPTOR, NUCLEAR LOCALIZATION SIGNAL, 2 ARMADILLO REPEATS, AUTONHIBITION, INTRASTERIC | NÚCLEAR IMPORT RECEPTOR KARYOPHERIN ALDHA, NÚCLEAR IMPORT RECEPTOR, NÚCLEAR LOCALIZATION SIGNAL, 2 ARMADILLO REPEATS, AUTONHIBITION, INTRASTERIC | STRUCTURAL PROTEIN ARMADILLO REPEAT, BETA-CATENIN, STRUCTURAL PROTEIN | ARMADILLO REPEAT ARMADILLO REPEAT, BETA-CATENIN, CYTOSKELETON | ARMADILLO REPEAT ARMADILLO REPEAT, BETA-CATENIN, CYTOSKELETON | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGMIN, C2-DOMAIN, EXOCYTOSIS, NEUROTRANSMITTER, 2 RELEASE, ENDOCYTOSIS/EXOCYTOSIS | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGMIN, C2-DOMAIN, EXOCYTOSIS, NEUROTRANSMITTER 2 RELEAS, ENDOCYTOSIS/EXOCYTOSIS |
|------------------|--|--|--|--|---|---|---|--|--|
| Coumpound | CHAIN: A, B; MYC PROTO- ONCOGENE PROTEIN; CHAIN: C, D, E, P; | KARYOPHERIN ALPHA; CHAIN: A, B; MYC PROTO- ONCOGENE PROTEIN; CHAIN: C, D. E. P. | IMPORTIN ALPHA; CHAIN: A; | Importin Alpha; chain: A; | BETA-CATENIN; CHAIN: NULL; | BETA-CATENIN; CHAIN: NULL; | BETA-CATENIN, CHAIN: NULL; | SYNAPTOTAGMIN I, CHAIN: A; | SYNAPTOTAGMIN I, CHAIN: A; |
| SeqFold score | | | 52.47 | | | | | | |
| PMF | | 0.17 | | _ | 86:0 | 0.94 | 0.75 | _ | 1 |
| Verify | | 0.03 | | 0.55 | 0.26 | 0.3 | 0.21 | 0.41 | 0.59 |
| PSI- BLAST | | 5.40E-10 | 1.40E-51 | 1.40E-51 | 3.60E-39 | 1.30E-29 | 5.40E-31 | 2.60E-39 | 3.60E-24 |
| End | | 347 | 344 | 343 | 347 | 336 | 347 | 265 | 264 |
| Start | | 233 | - | ٧. | . 56 | _ | 89 | 140 | 143 |
| Chain ID | | V | ∢ | ∢ | | | | 4 | ٧ |
| PDB CD | | ped lee4 | lial | Iial | 2bct | 3bct | 3bct | Ibyn | lbyn |
| SEQ NO: DE | | 777 | 111 | 111 | 111 | 111 | 11.1 | 677 | 971 |

| | | | | | | _ | | | | , | | T |
|----------------|--|--|---|---|--|---|--|---|---|---|--|---|
| PDB annotation | ENDOCYTOSIS/EXOCYTOSIS BETA SANDWICH, CALCIUM 10N, C2 DOMAIN | ENDOCYTOSIS/EXOCYTOSIS BETA SANDWICH, CALCIUM ION, C2 DOMAIN | | | - | | COMPLEX (ZINC FINGERIDNA) COMPLEX (ZINC FINGERIDNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGERIDNA) COMPLEX (ZINC FINGERIDNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGERIDNA) COMPLEX (ZINC FINGERIDNA), ZINC FINGER, DNA-BINDING PROTEIN | CONTRACTILE LIM DOMAIN, CRP, NMR, MUSCLE DIFFERENTIATION. CONTRACTILE | SIGNALLING PROTEIN BINDING PROTEIN, CYTOKINE, SIGNALLING PROTEIN | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX |
| Coumpound | SYNAPTOTAGMIN III; CHAIN: A; | SYNAPTOTAGMIN III; CHAIN: A; | CALCIUM/PHOSPHOLIPID BINDING PROTEIN SYNAPTOTAGMIN I (FIRST C2 DOMAIN) (CALB) IRSY 3 | CALCIUM/PHOSPHOLIPID BINDING PROTEIN SYNAPTOTAGMIN I (FIRST C2 DOMAIN) (CALB) IRSY 3 | CALCIUMPHOSPHOLIPID BINDING PROTEIN SYNAPTOTAGMIN I (FIRST C2 DOMAIN) (CALB) IRSY 3 | | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | CRP1; CHAIN: A; | TUMOR NECROSIS PACTOR RECEPTOR: CHAIN: A, B: | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; |
| SeqFold | | | 130.23 | | | | 10.71 | | | 58.15 | 57.16 | |
| PMF | - | - | | _ | _ | | | 0.03 | 90:0 | | | |
| Verify | 0.51 | 0.43 | | 0.35 | 0.56 | | | -0.31 | -0.2 | | | 0.32 |
| PSI- BLAST | 2.60E-73 | 9.00E-55 | 2.60E-41 | 2.60E-41 | 3.60E-24 | | 7.20E-31 | 7.20E-22 | 3.60E-26 | 7.80E-13 | 0.00026 | 3.60E-50 |
| End | 376 | 387 | 566 | 264 | 264 | | 227 | 16 | 691 | 277 | 981 | 197 |
| Start | 140 | 143 | 136 | 140 | 143 | | 145 | 19 | 95 | 88 | 10 | 116 |
| Chain | A | A | | | | | A | Ą | V | Ą | ¥ | င |
| EDB CI | 1dqv | Idqv | Irsy | lısy | Irsy | | lalh | lath | lalh | 168t | lext | lme y |
| S a S | <i>6LL</i> | <i>6LL</i> | 611 | 611 | 611 | | 783 | 783 | 783 | 783 | 783 | 783 |

| | _ | | | | | | | | | | | | | | | _ | | | | _ | | | | | | _ | | | _ | | | |
|------------------|-------------------|---|--|--------------------------------|-----------------------|----------------------------|-------------------|---|--------------------------------|----------------------------|-------------------|--------------------------------|----------------------|-----------------------------|-------------------|--------------------------------|-----------------------|--------------------------------|----------------------------|-------------------|--------------------------------|-------------------------------|---|-------------------|--------------------------------|-----------------------|---------------------------|-------------------|-------------------------|-------------------------|----------------------|---------------------------------|
| PDB annotation | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | PINGER, PROTEIN-DINA | CDVCTA1 CTD11CTTDE COMBLEY | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | INTER ACTION PROTEIN DESIGN 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, FROI EIN-UNA | COVETAL STRICTION CONTROL | (ZINC FINGER/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX | REGITLATION/DNA) RNA | POLYMERASE III, 2 TRANSCRIPTION |
| Coumpound | | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | rkolein; chain: c, r, c; | | DNA; CHAIN: A, B, D, E; | PROTEIN: CHAIN: C. F. G. | | | DNA; CHAIN: A, B, D, E; | DEOTERI CHARLO E O | ricotems, circuit. C, F, C, | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | | DNA; CHAIN: A, B, D, E; | PROTEIN: CHAIN: C P. G. | (C) (C) (C) (C) (C) (C) (C) (C) (C) (C) | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | |
| SeqFold score | | | | | | | | 92.4 | | | | | | | | | | | | | | | | | | | | | 87.93 | | | |
| PMF | | - | | _ | | | | | | | | 0.03 | | | | _ | | | | | 0.03 | | | | 0.74 | | | | | | | |
| Verify score | | 0.54 | | 0.47 | | | | | | | | -0.15 | | | | 0.43 | | | | , | -0.51 | | | | 80.0 | | | | | | | |
| PSI- BLAST | | 3.60E-50 | | 1.30E-50 | | | | 1.30E-50 | | | | 3.60E-39 | | | | 1.80E-46 | | | | 1 | 3.40E-42 | | | | 1.10E-45 | | | | 1.30E-58 | | | |
| End AA | | 225 | | 253 | | | | 254 | | | | 16 | | | | 276 | | | | | <u>4</u> | | | | 691 | | | | 275 | | | |
| Start AA | | 144 | | 172 | | | | 172 | | | | 18 | | | | 200 | | | | ş | 8 | | | | 8 | | | | 116 | | | |
| Chain ID | | ပ | | ပ | | | | υ | | | | ပ | | | | ပ | | | | , | د | | | | b | | | | ¥ | | | |
| PDB DD | | J me | | Ine Ine | <u>,</u> | | | e , | , | | | lme | <u>~</u> | | | Ime | ^ | | | 1 | Ë, | ` | | | lle : | >- | | | 911 | | | |
| SEQ No: | | 783 | | 783 | _ | | | 783 | | | | 783 | | | | 783 | | | | ŝ | \$ | | | | 783 | | | | 783 | | | |

| PDB annotation | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, INITIATOR FLEMENT VY1 ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGIT ATTOMONA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG I; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | ONTHE TOTAL | REGIT ATTONONALYNG-YANG 1: | TRANSCRIPTION INITIATION. | INITIATOR ELEMENT, YYI, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | COMPLEX ONLY PRIDRIC | PROTEIN/DNA) FIVE-ENIGEP GI 1: GI 1 | משטיים של איני היינים איניים של הייניים הייניים הייניים היינים הייניים היינים הייניים היינים היי | ZINC FINGER, COMPLEX (DNA- | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI: GLI. | ZINC FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER COMPI EX CONA. | BINDING PROTEIN/DNA) |
|------------------|---------------------------------|---|---|------------------------|------------------------|------------------------------|---|-----------------------------|---|------------------------|------------------------------|---------------------------|--------------------------------|-----------------------------|------------------------|---|----------------------------|---------------------------|--------------------------------|-----------------------------|------------------------|--------------------------|-------------------------------------|--|----------------------------|---------------------------|------------------------------------|----------------------------|----------------------|---------------------------|---|----------------------|
| Coumpound | | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; | CHAIN: A, B; | | YY1: CHAIN: C: ADENO- | ASSOCIATED VIRUS P5 | CHAIN: A. B. | | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | VVI. CUARI, C. ADENO | ASSOCIATED VIRIES PS | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | ZINC BINGED PROTEIN CLIT | CHAIN: A: DNA: CHAIN: C | , | á | ZINC FINGER PROTEIN GLI1: | CHAIN: A; DNA; CHAIN: C, | ď | | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, D: | |
| SeqFold score | | 85.55 | | | | | | | | | | | | | | | | | | | | 24 77 | 77.00 | | | | | | | | | |
| PMF score | | | | | 0.87 | | | | | _ | | | | | | 0.46 | 2 | | | | | | | | | _ | | | | 6.0 | | |
| Verify score | | | | | 0.1 | | | | | -0.02 | | | | | | 51.0 | 7 | | | | | | | | | 0.14 | | | | 0.23 | | |
| PSI- BLAST | | 3.90E-51 | | | 9.10E-47 | | | | | 3.90E-51 | | | | | | 3 KOF.32 | 3.000.0 | | | | | 3 90F-59 | 2000 | | | 3.90E-59 | | | | 1.30E-56 | | |
| End AA | | 526 | | | 225 | | | | | 254 | | | | | | 101 | | | | | | 255 | } | | | 255 | | | | 792 | | |
| Start AA | | 116 | | | 121 | | | | | 149 | | | | | | 70 | ? | | | | | 911 | : | | | 117 | | | | 145 | | |
| Chain 1D | | o | | | S | | | | | ပ | | | | | | ر | , | | | | | A | | | | Ą | | | | ∢ | | |
| PDB ID | | Tebd | | | lubd | | | | | Inpd Inpd | | | | | | Pale | 3 | | | | | 2gli | . | | | 2gli | | | | - 78H | | |
| S e S | | 783 | | | 783 | | | | | 783 | | | | | | 783 | ! | | | | | 783 | | | | 783 | _ | | - | 2 | | |

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| PDB annotation | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GIJ; GLJ, ZINC FINGER, COMPLEX (DNA-BINDING PROTEIN/DNA) | TRANSFERASE ATK. AMGX1. BPK: | TYROSINE KINASE, X-LINKED AGAMMAGLOBULINEMIA, XLA, BTK, SH3 2 DOMAIN, TRANSFERASE | COMPLEX (ADAPTOR PROTEINPETIDE) ASH, GROWTH PACTOR RECEPTOR-BOIND PROTEIN 2; COMPLEX (ADAPTOR PROTEINPETIDE), SHJ DOMAIN, 2 GUANINEAVICLEOTIDE RELEASING FACTOR | COMPLEX (TRANSFERASE/PEPTIDE) COMPLEX (TRANSFERASE/PEPTIDE), SIGNAL TRANSDUCTION, 2 SH3 DOMAIN | COMPLEX (SIGNAL TRANSDUCTION/PEPTIDE) COMPLEX (SIGNAL TRANSDUCTION/PEPTIDE), SH3 DOMAIN | SIGNAL TRANSDUCTION ADAPTOR SH2, SH3 IGRI 14 | CIRCULAR PERMUTANT PWT; CIRCULAR PERMUTANT, SH3 DOMAIN, CYTOSKELETON | CYTOSKELETON CYTOSKELETON, MEMBRANE, SH3 DOMAIN | SIGNAL TRANSDUCTION PROTEIN SRC-HOMOLOGY 3 (SH3) DOMAIN, PEPTIDE-BINDING PROTEIN, ISEM 18 2 GUANINE NUCLEOTIDE EXCHANGE FACTOR ISEM 19 | | ENDOCYTOSIS/EXOCYTOSIS NSECI; PROTEIN-PROTEIN COMPLEX, MULTI-SUBUNIT |
| Coumpound | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | BRUTON'S TYROSINE | KINASE; CHAIN: NULL; | GRB2; CHAIN: A; SOS; CHAIN: B; | ABL TYROSINE KINASE; CHAIN: A, C, B, G; PEPTIDE P41; CHAIN: B, D, F, H; | GRB2; CHAIN: A; SOS-1; CHAIN: B; | GROWTH FACTOR BOUND PROTEIN 2; 1GRI 5 CHAIN: A, B; 1GRI 6 | ALPHA SPECTRIN; CHAIN: NULL; | ALPHA II SPECTRIN; CHAIN: A; | SEM-5: ISEM 3 CHAIN: A, B; ISEM 3 IO-RESIDUE PROLINE-RICH PEPTIDE FROM MSOS ISEM 8 CHAIN: C, D ISEM 10 | | SYNTAXIN BINDING PROTEIN 1; CHAIN: A; SYNTAXIN 1A; CHAIN: B; |
| SeqFold score | | | | | | | | | | | | |
| PMF | 0.1 | 8.0 | | 0.83 | 0.25 | 0.87 | 0.12 | 0.59 | 12.0 | 0.59 | | 0.01 |
| Verify score | -0.43 | 0.42 | | 0.35 | 0.08 | 0.4 | 0.12 | 0.2 | -0.25 | 0.21 | | -0.67 |
| PSI- BLAST | 3.60E-26 | 1.00E-09 | | 2.60E-11 | 3.90E-10 | 9.10E-12 | 1.80E-09 | 2.60E-11 | 1.30E-10 | 5.40E-11 | | 1.00E-05 |
| End | 140 | 403 | | 402 | 403 | 403 | 400 | 403 | 403 | 400 | | 281 |
| Start | 26 | 340 | | 348 | 350 | 348 | 343 | . 344 | 349 | 349 | | 160 |
| Chain D | V | | | < | ⋖ | ∢ | ∀ | | A | V | | æ |
| 20 E | 2gli | law | ≽ | laze | 1bbz | 1gbq | irgi | Ipwt | 1qk w | Isem | | ldnl |
| 8 8 8 8 | 783 | 784 | | 784 | 784 | 784 | 784 | 784 | 784 | 784 | | 785 |

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|------------------|---|---|----------------|---|---|--------------------------------------|--|--|----------------------------|---------------------------------------|--|---|--|---|----------------------|---|-----------------|---|--|
| PDB annotation | | HALOPEROXIDASE BROMOPEROXIDASE L, HALOPEROXIDASE L, HALOPEROXIDASE L, | OXIDOREDUCTASE | HALOPEROXIDASE CHLOROPEROXIDASE A1, HALOPEROXIDASE A1; HALOPEROXIDASE, OXIDOREDUCTASE | HALOPEROXIDASE HALOPEROXIDASE F; HALOPEROXIDASE, OXIDOREDUCTASE, PROPIONATE COMPLEX | HALOPEROXIDASE HALOPEROXIDASE A2, | CHLOROPEROXIDASE A2; HALOPEROXIDASE | OXIDOREDUCTASE, PEROXIDASE, ALPHA/BETA 2 HYDROLASE FOLD, | HYDROLASE BPHD; HYDROLASE, | PCB DEGRADATION | HYDROLASE A/B HYDROLASE FOLD, DEHALOGENASE I-S BOND | HYDROLASE TRIACYLGLYCEROL- | CRYSTALLOGRAPHY, 2 | rseudomoinadaceae, Ox Tanion, CIS-PEPTIDE, HYDROLASE | HYDROLASE HYDROLASE, | ALPHA/BETA HYDROLASE FOLD, EPOXIDE DEGRADATION 2 | EPICHLOROHYDRIN | HYDROLASE HOMODIMER, ALPHA/BFTA HYDROLASE FOLD | DISUBSTITUTED UREA 2 INHIBITOR |
| Coumpound | | CHLOROPEROXIDASE L; CHAIN: A, B, C; | | BROMOPEROXIDASE A1; CHAIN: NULL; | CHLOROPEROXIDASE F, CHAIN: NULL; | BROMOPEROXIDASE A2; CHAIN: NULL; | | | 2-HYDROXY-6-0XO-6- | PHENYLHEXA-2,4- DIENOATE CHAIN: A; | HALOALKANE DEHALOGENASE; 1- CHLOROHEXANE CHAIN: A; | TRIACYLGLYCEROL HYDROI ASE: CHAIN: NIII I:- | יייים בייים ביים בייים ב | | SOLUBLE EPOXIDE | HYDROLASE; CHAIN: A, B, C, D: | | EPOXIDE HYDROLASE; | (a (a (a (a (a (a (a (a (a (a (a (a (a (|
| SeqFold | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.07 | | 0.05 | 0.22 | 0.28 | | | 18.0 | | 66'0 | 0.03 | | | 0.52 | | | 0.15 | |
| Verify | | -0.21 | | -0.13 | -0.12 | 0.14 | | | -0.02 | | 0.35 | 60:0 | | | 0.23 | | | | |
| PSI- BLAST | | 5.40E-45 | | 1.10E-38 | 7.20E-39 | 1.30E-39 | | | 5.40E-41 | | 1.80E-40 | 3.60E-11 | | | 5.40E-38 | | | 1.10E-37 | |
| End | | 258 | | 257 | 258 | 258 | | | 247 | | 257 | 203 | | | 256 | | | 258 | |
| Start | | 1 | | 6 | 7 | 7 | | | 17 | | 13 | 25 | | | | | | 4 | |
| Chain ID | | ¥ | | | | | | | A | | ٧ | | | | A | | | 4 | |
| EDB CD | | 1a88 | | 1a8q | 1a8s | 뎚 | | | lc4x | | lcqw | Icv | | | lehy | | | 뚕 | |
| SEQ ID NO: | | 786 | | 786 | 984 | 786 | | | 786 | | 786 | 786 | | | 982 | | | 982 | |

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|------------------|--|----------------------------------|---|--|--|--|---|---|--|---|---|--|
| PDB annotation | HYDROLASE HOMODIMER, ALPHA/BETA HYDROLASE FOLD, DISUBSTITUTED UREA 2 INHIBITOR | HYDROLASE LIPASE | | HYDROLASE PSEUDOMONADACEAE, CIS-PEPTIDE, CLOSED CONFORMATION, 2 HYDROLASE, LID | HYDROLASE ALPHA BETA HYDROLASE FOLD, PROLINE, PROLYL AMINOPEPTIDASE, 2 SERRATIA, IMINOPEPTIDASE | LIPASE LIPASE, HYDROLASE, PSEUDOMONADACEAE, COVALENT INTERMEDIATE, 2 TRIGLYCERIDE ANALOGUE, ENANTIOSELECTIVITY | | SIGNAL TRANSDUCTION SIGNAL TRANSDUCTION, SOS, PLECKSTRIN HOMOLOGY (PH) DOMAIN | SIGNAL TRANSDUCTION PROTEIN | TRANSPORT PROTEIN RHO-GTPASE EXCHANGE FACTOR, TRANSPORT PROTEIN | TRANSPORT PROTEIN RHO-CTPASE EXCHANGE FACTOR, TRANSPORT PROTEIN | GENE REGULATION SON OF SEVENLESS PROTEIN; GUANINE NUCLEOTIDE EXCHANGE FACTOR, GENE REGULATION |
| Coumpound | EPOXIDE HYDROLASE; CHAIN: A, B; | LIPASE, GASTRIC, CHAIN: A, B; | HYDROLASEICARBOXYLIC ESTRAASD.LINASE (E.C.3.1.3) COMPLEXED WITH COLLEASE AND INHERITED ILPB 3 BY UNDECANE PHOSPHONATE METHYL ESTRE (TWO CONFORMATIONS) ILPB 4 | TRIACYLGLYCERÔL HYDROLASE; CHAIN: D; TRIACYLGLYCERÔL HYDROLASE; CHAIN: E; | PROLYL AMINOPEPTIDASE; CHAIN: A; | TRIACYL-GLYCEROL- HYDROLASE; CHAIN: D, E; | | SOSI; CHAIN: NULL; | BETA-SPECTRIN; 1BTN 4 CHAIN: NULL; 1BTN 5 | PIX; CHAIN: A; | PIX; CHAIN: A; | HUMAN SOS 1; CHAIN: A; |
| SeqFold score | | | | | | | | | | | | |
| PMF | 0.13 | 0 | 0 | -0.03 | 0 | 0.01 | | 0.49 | _ | 68:0 | 9.0 | 96:0 |
| Verify score | -0.11 | -0.32 | -0.29 | 0.1 | -0.16 | -0.09 | | 0.32 | 0.39 | -0.25 | -0.46 | 0.1 |
| PSI- BLAST | 1.10E-37 | 1.60E-07 | 1.40E-06 | 3.60E-11 | 1.60E-28 | 1.60E-11 | | 1.20E-23 | 9.00E-09 | 2.60E-41 | 7.20E-23 | 1.80E-16 |
| End | 258 | 121 | 149 | 203 | 242 | 191 | | 276 | 819 | 463 | 462 | 570 |
| Start AA | 14 | 2 | 30 | 25 | | 25 | | 462 | 728 | 197 | 267 | 261 |
| Chain | В | ¥ | я | Q | ¥. | D | | | | 4 | ∢ | ¥ |
| aga a | lek! | lhlg | 1lpb | lqge | 1qtr | 4lip | | lawe | lbtn | lbyl | lby1 | ldbh |
| S e S | 786 | 786 | 786 | 786 | 786 | 786 | | 788 | 788 | 788 | 788 | 788 |

| PDB annotation | GENE REGULATION SON OF SEVENLESS PROTEIN; GUANINE NUCLEOTIDE EXCHANGE FACTOR, GENE REGULATION | CYTOSKELETON | TRANSFERASE HRS; HRS, VHS, FYVE, ZINC FINGER, SUPERHELIX | SIGNALING PROTEIN 11 ALPHA- HELICES | SIGNALING PROTEIN DAPPI, PHISH, BAMAZ, PLEKSTRIN, PHOSPHONOSITIDES, INOSIO. TETRAKISPHOSPHATE 2 SIGNAL TRANSDUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN DAPPI, PHISH, BAMAZ, PLEKSTRIN, PHOSPHONOSITIDES, NOSITOL TETRAKUSPHOSPHATE 2 SIGNAL TRANSDUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN DAPPI, PHISH, BAMAZ, PLECKSTRIN, PHOSPHONOSITIDES, INOSITO, TETRAKISPHOSPHATE 2 SIGNAL TRANSDUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN DAPPI, PHISH, BAMAZ, PLEKSTRIN, PHOSPHOINOSITIDES, INOSITO TETRAKISPHOSPHATE 2 SIGNAL TRANSDUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN ARFI GUANINE NUCLEOTIDE EXCHANGE FACTOR AND PH DOMAIN | SIGNALING PROTEIN ARFI GUANINE NUCLEOTIDE EXCHANGE FACTOR AND PH DOMAIN |
|------------------|--|--|---|--|--|--|--|---|---|---|
| Coumpound | HUMAN SOS I; CHAIN: A; | BETA-SPECTRIN; IDRO 6 CHAIN: NULL; IDRO 7 | HEPATOCYTE GROWTH FACTOR-REGULATED TYROSINE CHAIN: A; | RHO-GEF VAV; CHAIN: A; | DUAL ADAPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | DUAL ADAPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | DUAL ADAPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | DUAL ADAPTOR OF PHOSPHOTYROSINE AND 3- CHAIN: A; | GRP1; CHAIN: A; | GRP1; CHAIN: A; |
| SeqFold score | | | | | | | | | | |
| PMF | _ | 0.21 | - | | 0.94 | 0.29 | 0.99 | 0.98 | 0.21 | 0.98 |
| Verify score | 0.12 | 0.22 | 0.07 | 0.14 | 0.52 | 4.0- | 0.63 | 19.0 | -0.18 | 0.27 |
| PSI- BLAST | 7.80E-58 | 9.10E-09 | 9.00E-11 | 5.40E-24 | 3.60E-11 | 1.00E-09 | 2.60E-18 | 1.80E-11 | 9.10E-08 | 1.10E-15 |
| End | 576 | 820 | 674 | 454 | 816 | 574 | 817 | 816 | 574 | 821 |
| Start AA | 263 | 736 | 819 | 260 | 726 | 484 | 917 | 227 | 484 | 725 |
| Chain ID | ¥ | | Ą | V | V | ٧ | ∢ | ¥ | A | ٧ |
| PDB CI | 1dbh | 1dro | ldvp | 15x | Ifao | 1108 | 1168 | 1fb8 | Ifgy | 1fgy |
| SEQ No. | 788 | 882 | 884 | 788 | 788 | 788 | 788 | 788 | 788 | 788 |

| PDB annotation | SIGNALING PROTEIN ARFI GUANINE NUCLEOTIDE EXCHANGE FACTOR AND PH DOMAIN | | SIGNAL TRANSDUCTION IRS-1; BETA-SANDWHICH, SIGNAL TRANSDUCTION | TRANSPORT PROTEIN FYVE DOMAIN, ENDOSOME MATURATION, INTRACELLULAR TRAFFICKING, 2 TRANSPORT PROTEIN | COMPLEX (GTP-BINDING/EFFECTOR) RAS-RELATIB PROTERN RABBA; COMPLEX (GTP-BINDING/EFFECTOR), G PROTEIN EFFECTOR, RABCDR, 2 SYNAFTIC EXOCYTOSIS, RAB ROTEIN, RABBA, RABBAHLIN | RECEPTOR RECEPTOR, SIGNAL TRANSDUCER OF IL-6 TYPE CYTOKINES, THIRD 2 N-TERMINAL DOMAIN, TRANSMEMBRANE, GLYCOPROTEIN | RECEPTOR RECEPTOR, SIGNAL TRANSDUCER OF IL-6 TYPE CYTOKINES, THIRD 2 N-TERMINAL DOMAIN, TRANSMEMBRANE, GLYCOPROTEN | RECEPTOR RECEPTOR, SIGNAL TRANSDUCER OF IL-6 TYPE CYTOKINES, THIRD 2 N-TERMINAL DOMAIN, TRANSMEMBRANE, GLYOOPROTEIN |
|-----------------|---|--|--|---|---|---|--|---|
| Coumpound | GRP1; CHAIN: A; | PHOSPHORYLATION PLECKSTRIN N-TERMINAL PLECKSTRIN N-TERMINAL PLECKSTRIN HOMOLOGY DOMAIN) MUTANT IPLS 3 WITH LEG GLU (HIS)6 ADDED TO THE C TERMINUS IPLS 4 (INS(GIOS- LEBHHRHIN) (NAM, 25 STRUCTURES) IPLS 5 | INSULIN RECEPTOR SUBSTRATE 1; CHAIN: A, B; | PHOSPHATIDYLINOSITOL-3- PHOSPHATE BINDING FYVE CHAIN: A; | RAB-3A; CHAIN: A; RABPHILIN-3A; CHAIN: B; | GPI30; CHAIN: NULL; | GP130; CHAIN: NULL; | GP130; CHAIN: NULL; |
| SeqFold | | | | | | | | |
| PMF | 90:06 | 0.93 | 0.76 | 0.94 | 0.1 | 0:00 | 0.13 | -0.01 |
| Verify score | -0.15 | 1.0 | 0.64 | 0.04 | 0.11 | 80.0 | -0.09 | 0.14 |
| PSI- BLAST | 7.80E-16 | 1.80E-11 | 3.60E-05 | 7.20E-08 | 3.90E-21 | 1.10E-08 | 3.60E-11 | 7.20E-11 |
| End | 814 | 819 | 918 | 671 | 674 | 360 | 477 | 580 |
| Start | 729 | 728 | 725 | 620 | 290 | . 588 | 387 | 484 |
| Chain | 4 | | ٧ | ٧ | В | | | |
| PDB ID | lfgy | l pis | 1998 | lvfy. | 1zbd | 8jd1 | 15j8 | 1bj8 |
| S B S | 788 | 788 | 788 | 788 | 788 | 789 | 789 | 789 |

| PDB annotation | CONNECTIN A71, CONNECTIN; TITIN, CONNECTIN, FIBRONECTIN TYPE III | CONNECTIN A71, CONNECTIN; TITIN, CONNECTIN, FIBRONECTIN TYPE III | SIGNALING PROTEIN CYTOKINE RECEPTOR, GLYCOPROTEIN 130, GP130, INTERLEUKINE 6 2 RECEPTOR BETA SUBUNIT, SIGNALING PROTEIN | SIGNALING PROTEIN CYTOKINE RECEPTOR, GLYCOPROTEIN 130, GP130, INTERLEUKINE 6 2 RECEPTOR BETA SUBUNIT, SIGNALING PROTEIN | SIGNALING PROTEIN CYTOKINE RECEPTOR, GLYCOPROTEIN 130, GP130, INTERLEUKINE 6 2 RECEPTOR BETA SUBUNIT, SIGNALING PROTEIN | | HORMONEGROWTH FACTORHORMONE RECEPTOR 4- HELICAL BUNDLE, ALPHA HELICAL BUNDLE, TERNARY COMPLEX, FN 2 III DOMANNS, BETA SHEET DOMAINS, CYTOKINE-RECEPTOR COMPLEX | | | |
|-----------------|--|--|--|--|--|---|--|--|--|---|
| Coumpound | TITIN; CHAIN: NULL; | TITIN; CHAIN: NULL; | GP130; CHAIN: A, B; | GP130; CHAIN: A, B; | GP130; CHAIN: A, B; | NEURAL ADHESION MOLECULE DROSOPHILA MOLECULE DROSOPHILA NEUROGLIAN (CHYMOTRYPTIC FRAGMENT CONTAINING THE CERB 3 TWO AMINO THE CERB 3 TWO AMINO TYPE III REPEATS ICFB 4 RESIDUES 610 - 814) I CEPB 5 | PLACENTAL LACTOGEN; CHAIN: A; PROLACTIN RECEPTOR; CHAIN: B, C; | CELL ADHESION PROTEIN FIBRONECTIN CELL- ADHESION MODULE TYPE III-10 1FNA 3 | CELL ADHESION PROTEIN FIBRONECTIN CELL ADHESION MODULE TYPE III-10 1FNA 3 | CELL ADHESION PROTEIN FIBRONECTIN CELL- |
| SeqFold | | | | | | | | | | |
| PMF | 0.11 | 0.25 | 90:0 | -0.14 | -0.03 | 0.24 | 0.19 | 0.19 | 0.22 | 0.41 |
| Verify score | -0.31 | -0.02 | -0.19 | 0.09 | 0.11 | 0.03 | -0.26 | -0.14 | 0.04 | 0.07 |
| PSI- BLAST | 3.60E-07 | 3.60E-10 | 7.20E-21 | 9.00E-15 | 1.80E-18 | 1.80E-26 | 1.60E-14 | 3.60E-07 | 1.10E-11 | 1.30E-12 |
| End | 360 | 878 | 360 | 490 | 565 | 583 | 359 | 360 | 582 | 286 |
| Start | 288 | 485 | 195 | 288 | 386 | 385 | 196 | 295 | 492 | 504 |
| Chain | | | ¥ | ¥ | ¥ | | Ф | | | |
| PDB DD | Ibpv | Ibpv | Ibqu | lbqu | Ibqu | 1cfb | 116f | Ifna | lfna | Ifna |
| S e S | 789 | 789 | 682 | 789 | 789 | 789 | 789 | 682 | 789 | 789 |

| PDB annotation | | CELL ADHESION PROTEIN RGD, EXTRACELLILAR MATRIX IENF 18 | CELL ADHESION PROTEIN RGD, | CELL ADHESION PROTEIN RGD, | CELL ADHESION PROTEIN RGD, | HEPARIN AND INTEGRIN BINDING HEPARIN AND INTEGRIN BINDING | HEPARIN AND INTEGRIN BINDING HEPARIN AND INTEGRIN BINDING | HYDROLASE TYROSINE PHOSPHATEASE LAR PROTEIN | HYDROLASE TYROSINE PHOSPHATEASE, LAR PROTEIN | HYDROLASE TYROSINE PHOSPHATEASE LAR PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN, RGD, EXTRACELLIAR MATRIX, 2 HEPARPARNINMS GI YCOPPOTEIN | CELLANDESION PROTEIN CELL ADHESION PROTEIN, RGD, EXTRACELLULAR MATRIX, 2 HFPARIN-BINDING, GI, YCOPROTEIN | STRUCTURAL PROTEIN INTEGRIN, HEMIDESMOSOME, FIBRONECTIN, CARCINOMA, STRUCTURAL 2 PROTEIN | STRUCTURAL PROTEIN INTEGRIN, HEMIDESMOSOME, FIBRONECTIN, CARCINOMA, STRUCTURAL 2 PROTEIN | STRUCTURAL PROTEIN INTEGRIN, HEMIDESMOSOME, FIBRONECTIN, CARCINOMA, STRUCTURAL 2 PROTEIN | STRUCTURAL PROTEIN TENASCIN, |
|-----------------|---------------------------------------|---|----------------------------|----------------------------|----------------------------|---|--|--|---|--|--|--|---|--|---|------------------------------|
| Coumpound | ADHESION MODULE TYPE III-10 1FNA 3 | FIBRONECTIN; 1FNF 6 CHAIN; NULL: 1FNF 7 | FIBRONECTIN; IFNF 6 | FIBRONECTIN; IFNF 6 | FIBRONECTIN; IFNF 6 | FIBRONECTIN; CHAIN: A; | FIBRONECTIN; CHAIN: A; | LAR; CHAIN: A, B; | LAR; CHAIN: A, B; | LAR; CHAIN: A, B; | FIBRONECTIN; CHAIN: NULL; | FIBRONECTIN; CHAIN: NULL; | INTEGRIN BETA-4 SUBUNIT; CHAIN: A, B; | INTEGRIN BETA-4 SUBUNIT; CHAIN: A, B; | INTEGRIN BETA-4 SUBUNIT; CHAIN: A, B; | TENASCIN; CHAIN: A, B; |
| SeqFold | | | 120.84 | | | | | | | | | | | | | |
| PMF | | 0.51 | | 0.31 | -0.07 | 0.07 | 0.55 | _ | _ | _ | 0.16 | 0.09 | 0.1 | -1.41 | 0.92 | 0.18 |
| Verify score | | -0.02 | | -0.03 | 0.02 | 0.11 | 0.05 | 99.0 | 0.34 | 0.72 | 0.12 | -0.13 | 0.18 | 0.28 | 0.3 | 0.12 |
| PSI- BLAST | | 5.40E-39 | 5.40E-39 | 9.00E-38 | 9.00E-39 | 1.10E-19 | 7.20E-32 | 0 | 3.60E-81 | 0 | 5.40E-23 | 1.80E-25 | 1.10E-17 | 1.40E-25 | 2.60E-29 | 9.00E-17 |
| End AA | | 582 | 288 | 674 | 752 | 473 | 673 | 1462 | 1164 | 1462 | 474 | 282 | 478 | 588 | 584 | 480 |
| Start AA | | 192 | 194 | 288 | 386 | 961 | 389 | 893 | 782 | 924 | 292 | 388 | 290 | 388 | 390 | 292 |
| Chain D | | | | | | V | V | ¥ | В | м | | | ٧ | ¥ | ¥ | Ą |
| PDB | | 1fif | IBF | ĵij. | μĘ | 重 | Iţii | llar | llar | Ilar | llmfi | 1mfn | lqg3 | 19,83 | Egp1 | Ig B |
| SEQ NO: | | 789 | 789 | 789 | 789 | 789 | 789 | 789 | 789 | 789 | 789 | 789 | 789 | | 789 | 789 |

| | | | | | | , | | | | | | |
|------------------|--|--|--|--|---|---|---|---|---|--|---|--|
| PDB annotation | FIBRONECTIN TYPE-III, HEPARIN, EXTRACELULAR 2 MATRIX, ADHESION, FUSION PROTEIN, STRUCTURAL PROTEIN | STRUCTURAL PROTEIN TENASCIN, FIBRONECTIN TYPE-11I, HEPARIN, EXTRACELLULAR 2 MATRIX, ADHESION, FUSION PROTEIN, STRICTURAL PROTEIN | RECEPTOR DI; RECEPTOR, PHOSPHATASE, SIGNAL, TRANSDUCTION, ADHESION, 2 HYDROLASE | RECEPTOR DI, RECEPTOR, PHOSPHATASE, SIGNAL TRANSDUCTION, ADHESION, 2 HYDROLASE | | | | IMMUNE SYSTEM CD32; RECEPTOR, FC. CD32. IMMUNE SYSTEM | PROTEIN BINDING ED-B, FIBRONECTIN, TYPEIU DOMAIN, ANGIOGENESIS, PROTEIN 2 BINDING | PROTEIN BINDING ED-B, FIBRONECTIN, TYPEIII DOMAIN, ANGIOGENESIS, PROTEIN 2 BINDING | TYROSINE PHOSPHATASE SYP, SHPTP-2; TYROSINE PHOSPHATASE, INSULIN SIGNALING, SH2 PROTEIN | |
| Coumpound | | TENASCIN; CHAIN: A, B; | RECEPTOR PROTEIN TYROSINE PHOSPHATASE MU; CHAIN: A, B; | RECEPTOR PROTEIN TYROSINE PHOSPHATASE MU; CHAIN: A, B; | CELL ADHESION PROTEIN TENASCIN (THIRD FIBRONECTIN TYPE III REPEAT) ITEN 3 | CELL ADHESION PROTEIN TENASCIN (THIRD FIBRONECTIN TYPE III REPEAT) ITEN 3 | GLYCOPROTEIN FIBRONECTIN (TENTH TYPE 111 MODULE) (NMR, 36 STRUCTURES) 1TTF 3 | FC GAMMA RIIB: CHAIN: A; | FIBRONECTIN; CHAIN: A; | FIBRONECTIN; CHAIN: A; | SHP-2; CHAIN: A, B; | |
| SeqFold score | | | 405.81 | | | | | | | | | |
| PMF | | 0.41 | | - | 0.03 | 0.03 | 0.31 | -0.2 | 86:0 | 0.16 | 1 | |
| Verify score | | 0.32 | | 0.85 | 0.08 | 0.08 | 0.16 | 0.03 | 0.35 | 0.31 | 0.44 | |
| PSI- BLAST | | 1.30E-20 | 1.40E-89 | 1.40E-89 | 1.60E-07 | 1.30E-08 | 5.40E-13 | 1.40E-10 | 1.60E-05 | 1.80E-08 | 1.40E-72 | |
| End AA | | 584 | 1166 | 1165 | 584 | 584 | 582 | 163 | 480 | 584 | 1164 | |
| Start AA | | 390 | 688 | 168 | 487 | 502 | 485 | 27 | 391 | 490 | 835 | |
| Chain ID | | ٧ | ¥ | Ą | | | | ∢ | ∢ | ٧ | Y | |
| PDB ID | | 1qr4 | lrpm | Irpm | lten | lten | Ħ | 2fcb | 2fnb | 2fnb | 2shp | |
| SEQ NO: | | 789 | 789 | 789 | 789 | 789 | 789 | 789 | 789 | 789 | 789 | |

| PDB annotation | OXIDOREDUCTASE PDZ DOMAIN, NNOS, NITRIC OXIDE SYNTHASE | OXIDOREDUCTASE PDZ DOMAIN, NNOS, NITRIC OXIDE SYNTHASE | PEPTIDE RECOGNITION PEPTIDE RECOGNITION, PROTEIN LOCALIZATION | PEPTIDE RECOGNITION PEPTIDE RECOGNITION, PROTEIN LOCALIZATION | SIGNAL TRANSDUCTION PROTEIN | SIGNALING PROTEIN DAPPI, PHISH, | PHOSPHOINOSITIDES, INOSITOL TETRAKISPHOSPHATE 2 SIGNAL | TRANSDUCTION PROTEIN, ADAPTOR PROTEIN | SIGNALING PROTEIN ARFI GUANINE NUCLEOTIDE EXCHANGE FACTOR AND PH DOMAIN | CYTOKINE LCF, CYTOKINE, LYMPHOCYTE CHEMOATTRACTANT FACTOR, PDZ DOMAIN | OXIDOREDUCTASE BETA-FINGER | OXIDOREDUCTASE BETA-FINGER | MEMBRANE PROTEIN/OXIDOREDUCTASE BETA- FINGER, HETERODIMER | MEMBRANE PROTEIN/OXIDOREDUCTASE BETA- FINGER, HETERODIMER |
|------------------|---|---|---|---|--|---------------------------------|--|---------------------------------------|---|---|---|---|--|---|
| Coumpound | NEURONAL NITRIC OXIDE SYNTHASE; CHAIN: A; HEPTAPEPTIDE; CHAIN: B; | NEURONAL NITRIC OXIDE SYNTHASE; CHAIN: A; HEPTAPEPTIDE; CHAIN: B; | PSD-95; CHAIN: A; CRIPT; CHAIN: B; | PSD-95; CHAIN: A; CRIPT; CHAIN: B; | BETA-SPECTRIN; 1BTN 4 CHAIN: NULL; 1BTN 5 | DUAL ADAPTOR OF | CHAIN: A; | | GRP 1; CHAIN: A; | INTERLEUKIN 16; CHAIN: NULL; | NEURONAL NITRIC OXIDE SYNTHASE (RESIDUES 1- 130): CHAIN: A: | NEURONAL NITRIC OXIDE SYNTHASE (RESIDUES 1- 130): CHAIN: A: | ALPHA-I SYNTROPHIN (RESIDUES 77-171); CHAIN: A; NEURONAL NITRIC OXIDE SYNTHASE (RESIDIIES 1-130; CHAIN: B. | ALPHA-I SYNTROPHIN (RESIDUES 77-171), CHAIN: A; NEURONAL NITRIC OXIDE SYNTHASE |
| SeqFold score | 58.72 | | 57.29 | | | | | | | | | | 77.08 | |
| PMF | | 0.23 | | - | 9.04 | -0.13 | | | 0.05 | 0.43 | 66:0 | 0.94 | | _ |
| Verify score | | 0.46 | | 1.06 | -0.05 | 0.24 | | | -0.65 | 0.09 | 0.5 | 0.47 | | 0.87 |
| PSI- BLAST | 1.40E-11 | 1.40E-11 | 9.00E-16 | 9.00E-16 | 3.60E-10 | 5.40E-09 | | | 0.0052 | 3.60E-11 | 3.60E-10 | 2.60E-23 | 3.90E-23 | 3.90E-23 |
| End | 176 | 171 | 163 | 143 | 388 | 385 | | | 267 | 138 | 166 | 168 | 140 | 136 |
| Start AA | 48 | 22 | 45 | 49 | 299 | 295 | | | 661 | 27 | 5 4 | 95 | 24 | 26 |
| Chain ID | A | Ą | A | A , | | ¥ | | | A | | ٧ | Ą | ¥. | V |
| EDB CD | 1689 | 158q | 1be9 | 1be9 | lbtn | Ifao | | | Ifgy | 1116 | lqau | Iqau | Iqav | Iqav |
| SEQ No. | 793 | 793 | 793 | | 793 | 793 | | | | 793 | 793 | 793 | 793 | 793 |

| | | | _ | | _ | | | | _ | . – | | | , | | | | _ | | _ | _ | | |
|------------------|-----------------------------|---|---|---|-----------------------------|---------------------------|----------------------|---|--|---|-------------------------------|--|------------------------|--|--------------------------------|-------------------------------------|------------------|---------------------------|--------------|-------------------------|--------------------------------------|--|
| PDB annotation | | MEMBRANE PROTEINOXIDOREDUCTASE BETA- FINGER, HETERODIMER | | RNA-BINDING PROTEIN/RNA TRA PRE-MRNA; SPLICING REGULATION, RNP DOMAIN, RNA COMPLEX | GENE REGULATION/RNA POLY(A) | PROTEIN-RNA COMPLEX, GENE | REGULATION/RNA | | RNA BINDING PROTEIN RNA- BINDING DOMAIN | NUCLEAR PROTEIN HETEROGENEOTIS MICT EAD | RIBONUCLEOPROTEIN AI, NUCLEAR | FROIEIN, FINRNY, KED, KKM, KNF, RNA BINDING, 2 RIBONUCLEOPROTEIN | NUCLEAR PROTEIN | HEIEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN A1, NUCLEAR | PROTEIN, HNRNP, RBD, RRM, RNP, | KNA BINDING, 2 RIBONUCLEOPROTEIN | COMPLEX | (KIBONUCLEOPROTEIN/RNA) | | | | RNA BINDING PROTEIN RNA- BINDING DOMAIN |
| Coumpound | (RESIDUES 1-130); CHAIN: B; | ALPHA-I SYNTROPHIN (RESIDUES 77-17); CHAIN: A; NEURONAL NITRIC OXIDE SYNTHASE (RESIDUES 1-130); CHAIN: B; | | SXL-LETHAL PROTEIN; CHAIN: A, B; RNA (5'- K(P*GP*UP*UP*UP*UP*U P*UP*UP*UP*UP*UP. CHAIN: P, Q; | POLYDENYLATE BINDING | D. E. F. G. H. RNA (5'- | R(*AP*AP*AP*AP*AP*AP | *AP*AP*AP*A)-3'); CHAIN: M. N. O. P. O. R. S. T: | HU ANTIGEN C; CHAIN: A; | HNRNP AI; CHAIN: NULL; | | | HNRNP A1; CHAIN: NULL; | | | | UIA SPLICEOSOMAL | PROTEIN; TORN S CHAIN: A, | HAIRPIN (5'- | (AP*AP*UP*CP*CP*AP*UP*U | P* IURN II CHAIN: P, Q, R IURN I3 | MUSASHII; CHAIN: A; |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | |
| PMF score | | - | | 0.81 | 0.99 | | | | 0.71 | 9.63 | | | 66'0 | | | | 96'0 | | | | | 88.0 |
| Verify score | | 0.93 | | 0.84 | 0.41 | | | | 0.39 | 0.48 | | | 99.0 | | | | 0.55 | | | | | 0.82 |
| PSI- BLAST | | 3.60E-16 | | 1.80E-16 | 5.40E-18 | | | | 1.30E-15 | 9.00E-25 | | | 1.80E-15 | | | | 2.60E-15 | | | | | 1.60E-15 |
| End AA | | 139 | | 108 | 109 | | | | 105 | 103 | | | 107 | | | | 112 | | | | | 103 |
| Start AA | | 56 | | 33 | ∞ | | | - 0 | 34 | _ | | | 34 | | | | 33 | | | | | 35 |
| Chain | | ¥ | | ¥ | A | | | | ٧ | | | | | | | | ٧ | | | | | ¥ |
| eg a | | 1qav | | 167£ | lcvj | | | | 78pI | lhai | | | lhal | | | | Ium | | | | | 2mss |
| SEQ No ib | | 793 | | 794 | 794 | | | | 794 | 794 | | | 794 | | | | 794 | | | | | 794 |

| PDB annotation | RNA-BINDING DOMAIN RNA- BINDING DOMAIN, ALTERNATIVE SPLICING | COMPLEX (RIBONICLEOFROTEINDNA) HYRNP ALI, UPI, COMPLEX (RIBONICLEOFROTEINDNA), HETEROGENEGUS NICLEAR 2 RIBONICLEOFROTEIN AI | RNA BINDING DOMAIN RNA BINDING DOMAIN, RBB, RNA BERCORHTION MOTH, RRA, 2 SPLCING INHIBITOR, TRANSI, ATIONAL INHIBITOR, SEX 3 DETERMINATION, X CIRCOMOSOME DOSTAGE COMPENSATION | | COMPLEX (TRANSCRPTON REGULATIONONA) SREBE-14; STEROL REGULATORY ELEMENT BINDING PROTEIN, LASAGCHELIX- LOOP-HELIX-LEICING 2PPER, SREBF, TRANSCRIPTION 1 FACTOR, COMPLEX (TRANSCRIPTION | COMPLEX (TRANSCRPTION REGULATIONNYA SIRBPL-14; STEROL REGULATORY ELEMENT BINDING PROTEIN, 2 BASIC-HELIX- LOOP-HELIX-LEUGINE ZIPPER, SIRBP, TRANSCRPTION 5 PACTOR, COMPLEX (TRANSCRPTION | COMPLEX (DNA-BINDING PROTEIN; MAX, DNA BINDING, BASIC-HELIX-LOOP-HELIX-LEOCINE ZIPPER, 2 TRANSCHETTON FACTOR, COMPLEX ODA-BINDING PROTEIN/DNA. | COMPLEX (DNA-BINDING PROTEIN/DNA) UPSTREAM |
|-----------------|--|--|---|---|---|---|--|---|
| Coumpound | SEX-LETHAL PROTEIN; CHAIN: NULL; | HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN A1; CHAIN: A; IZ-NUCLEOTIDE SINGLE-STRANDED TELOMETRIC DIVA; CHAIN; B; | SEX-LETHAL; CHAIN: A, B, C; | | STEROL REGULATORY ELEMENT BINDING PROTEIN IA; CHAIN: A, B, C, D: DNA; CHAIN: E, F, G, H; | STEROL REGULATORY ELEMENT BINDING PROTEIN 14; CHAIN: 4, B, C, D; DNA; CHAIN: E, F, G, H; | MAX PROTEIN; CHAIN: A, C; DNA; CHAIN: B, D; | USF; CHAIN: A, B; DNA; CHAIN: C, D; |
| SeqFold | | | | | | | | |
| PMF | 89.0 | 0.23 | 96.0 | | 0.04 | 0.27 | -0.03 | 0.07 |
| Verify score | 0.31 | 0.68 | 0.61 | | 0.23 | 0.14 | 0.35 | -0.08 |
| PSI- BLAST | 1.80E-16 | 5.40E-30 | 5.40E-16 | | 2.60E-13 | 1.30E-15 | 9.00E-15 | 1.80E-13 |
| End | 801 | Ξ | 105 | | 131 | 119 | 119 | 115 |
| Start | 33 | - | 33 | 7 | . 65 | 55 | 57 | 35 |
| Chain ID | | ∢ | ∢ | | ٧ | м | ∢ | ٧ |
| PDB DD | 2sxl | 2up1 | 3sxl | | lam 9 | lam 9 | lan2 | lan4 |
| SEQ NO: DE | 794 | 794 | 794 | | 795 | 795 | 795 | 795 |

| PDB annotation | STIMULATORY FACTOR 1; USF, DNA BINDING, BASIC-HELLX, LOOP-HELLX, LEUCINE ZIPPER, 2 TRANSCRIPTION FACTOR, COMPLEX (DNA-BINDING PROTEIN/DNA) | COMPLEX (TRANSCRIPTION FACTOR MAX/DNA) TRANSCRIPTIONAL REGULATION, DNA BINDING, COMPLEX 2 (TRANSCRIPTION FACTOR MAX/DNA) | COMPLEX (TRANSCRIPTION FACTOR MAXODAA) TRANSCRIPTIONAL REGULATION, DNA BINDING, COMPLEX 2 (TRANSCRIPTION FACTOR MAXONA) | | COMPLEX (ZINC FINGERDNA) COMPLEX (ZINC FINGERDNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) ZINC |
|------------------|--|--|---|---|--|---|---|--------------------------------|
| Coumpound | | TRANSCRIPTION FACTOR MAX; CHAN: A, B; DNA (5'- D(*CP*AP*CP*CP*AP*CP*GP *TP*GP*GP*T)-3', CHAIN: C, D; | TRANSCRIPTION FACTOR MAX; CHANN: A. B. DNA (5'- D(*CP*AP*CP*AP*CP*GP *TP*GP*GP*T)-3', CHAIN: C, D. | TRANSCRIPTION ACTIVATIONDIA MYOD BASIG-HELIX (BHLI) DOMAIN IMDY 3 (RESIDUES IG. 166) MUTANT WHH CYS 135 REPLACED BY SIR IMDY 4 (CISS) COMPLEXED WITH DIA IMDY 5 (S. DI TP-CP-AP-AP-CP-AP-GP MDY 6 FOR THE CP-AP-AP-GP-AP-GP MDY 6 FOR THE CP-AP-AP-GP-AP-GP MDY 6 FOR THE CP-AP-AP-GP-AP-GP MDY 6 FOR THE CP-AP-AP-GP-AP-AP-GP MDY 6 FOR THE CP-AP-AP-AP-GP-AP-AP-GP MDY 6 FOR THE CP-AP-AP-AP-AP-GP-AP-AP-GP MDY 6 FOR THE CP-AP-AP-AP-AP-AP-GP-AP-AP-GP MDY 6 FOR THE CP-AP-AP-AP-AP-AP-AP-AP-GP MDY 6 FOR THE CP-AP-AP-AP-AP-AP-AP-AP-AP-AP-AP-AP-AP-AP | QGSR ZINC FINGER PEPTIDE, CHAIN: A; DUPLEX OLIGONUCLEOTIDE RINDING SITE: CHAIN: B C: | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B. C: | DNA; CHAIN: A, B, D, E; |
| SeqFold score | | | | | | | | |
| PMF score | | 0.17 | 0.05 | 0.11 | -0.19 | 0.55 | 0.42 | 89.0 |
| Verify score | | 90.0 | -0.17 | 0.15 | 0.07 | 0.24 | 0.31 | 0.14 |
| PSI- BLAST | | 3.60E-15 | 7.20E-15 | 1.40E-14 | 1.40E-22 | 3.60E-26 | 5.20E-32 | 5.40E-44 |
| End AA | | 611 | 119 | 4 | 405 | 433 | 434 | 433 |
| Start | | 53 | 55 | 8 | 327 | 353 | 357 | 352 |
| Chain ID | | Ą | B | _α | Ą | ∢ | ٧ | C |
| PDB ID | | lhlo | Ihlo |) y | lath | lalh | lalh | Ime |
| SEQ NO: | | 262 | 795 | 795 | 800 | 800 | 008 | 800 |

| PDB annotation | FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL, STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA NITERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA |
|------------------|---|---|--|--|--|--|--|--|--|
| Coumpound | CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER |
| SeqFold score | | | | | | | | | |
| PMF | | _ | - | _ | _ | _ | _ | - | _ |
| Verify score | | 0.49 | 0.45 | 0.52 | 0.52 | 0.48 | 0.45 | 0.15 | 0.19 |
| PSI- BLAST | | 1.80E-46 | 3.90E-48 | 2.60E-48 | 5.40E-47 | 9.00E-48 | 1.80E-48 | 9.00E-50 | 1.80E-50 |
| End AA | | 461 | 461 | 489 | 489 | 517 | 545 | 573 | 109 |
| Start | | 380 | 381 | 408 | 408 | 436 | | 492 | 520 |
| Chain | | ပ | U | o | ပ | ပ | ပ | ပ | ပ |
| PDB ED | 5 | Ime y | Jme y | Ime y | Jme y | Ime y | Ime y | y Ime | ıme v |
| Se o | | 008 | 008 | 008 | 800 | 800 | 008 | 008 | 80 |

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|------------------|---|---|-------------------|--|--|--------------------------------|-----------------------|--------------------------------|----------------------------|--------------------------------|-----------------------|--------------------------------|----------------------------|-------------------|--|--------------------------------|----------------------------|--------------------------------|-----------------------|--------------------------------|----------------------------|--------------------------------|-----------------------|--------------------------------|----------------------------|-------------------|--------------------------------|---|
| PDB annotation | INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | COMPLEX (ZINC PINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 |
| Coumpound | PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | DNA: CHAIN: A. B. D. E. | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | DNA: CHAIN: A. B. D. E. | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER | PROTEIN: CHAIN: C. F. G. | | DNA; CHAIN: A, B, D, E. | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | ٠ | DNA: CHAIN: A B D P. | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; |
| SeqFold score | | | | | | 107.23 | ! | | | | | | | 1 | | | | | | | | | | | | | | |
| PMF | | _ | | _ | | | | | | - | | | | | | | | _ | | | | - | | | | | _ | |
| Verify score | | 0.3 | | 0.21 | | | | | | 0.38 | | | | | 0.54 | | | 0.54 | | | | 0.41 | | | | | 0.19 | |
| PSI- BLAST | | 5.40E-51 | | 3.60E-51 | | 3.60E-51 | | | | 5.40E-51 | | | | | 1.20E-51 | | | 1.40E-50 | | | | 1.40E-50 | | | | | 9.00E-46 | |
| End AA | | 629 | | 657 | | 658 | | | | 685 | | | | | 713 | | | 713 | | | | 741 | | | | | 292 | |
| Start AA | | 548 | | 925 | | 576 | | | | 604 | | | | 1 | 632 | | | 632 | | | | 099 | | | | | 889 | |
| Chain . ID | | ပ | | ၁ | | U | | | | o | | | | , | | | | o | | | | S | | | | | υ υ | |
| PDB JD | | Jme y | | lme y | | Ime | ~ | | | m | ^ | | | l | e , | | | lme | ^ | | | Ime | ^ | | | 1 | e , | _ |
| SEQ NO: | | 008 | | 008 | | 008 | | | | 800 | | | | 000 | 8 | | | 800 | | | | 800 | | | | | 200 | |

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|------------------|--|--|--------------------------------|--|--------------------------------|--|--------------------|--|---------------------------------|--|--------------------|---------------------|---------------------------------|------------------------|-------------------------|--------------------|----------------------|---------------------------------|---------------------------------|-------------------------|-------------------------|----------------------|---------------------------------|---------------------------------|--|---------------------------|--------------------------------|-----------------------------|--------------------------------|------------------------|
| PDB annotation | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) TFIIIA; 5S GENE; NMR. TFIIIA, PROTEIN, DNA. | TRANSCRIPTION FACTOR, 5S RNA 2 | GENE, DNA BINDING PROTEIN, ZINC FINGER, COMPLEX 3 | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX | (TRANSCRIPTION | REGULATION/DNA), RNA DOI VMEDASE III 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION DEGIT ATTOMONA) COMPLEY | (TRANSCRIPTION | REGULATIONDNA), RNA | POLYMERASE III, 2 TRANSCRIPTION | COMMETS OF ANSCHOOLS | REGILATION/DNA) COMPLEX | (TRANSCRIPTION | REGULATION/DNA), RNA | POLYMERASE III, 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | KEGULATION/DNA) COMPLEX | REGULATION DNA). RNA | POLYMERASE III, 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION DECILI ATTOMINA) VINC VANC 1. | TRANSCRIPTION INITIATION. | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION |
| Coumpound | | TRANSCRIPTION FACTOR IIIA; CHAIN: A; 5S RNA GENE: CHAIN: E. F. | | | | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | | | TFIIIA; CHAIN: A, D; 5S | CHAIN: B. C. E. F. | | | TELLIA CITABLE A P. 60 | RIBOSOMAL RNA GENE: | CHAIN: B, C, E, F. | _ | | | TFIIIA; CHAIN: A, D; 5S | KIBUSOMAL KNA GENE; | Circile: 5, C, L, T, | | | YY1; CHAIN: C; ADENO- | INITIATOR ELEMENT DNA: | CHAIN: A, B; | | | YYI; CHAIN: C; ADENO- |
| SeqFold score | | | | | | | | | | | | | | 11.60 | 3 | | | | | | | | | | | | | | | |
| PMF | | -0.2 | | | | 0.54 | | | | _ | | | | | | | | | | _ | | | | | 0.43 | | | | | 96.0 |
| Verify score | | 0 | | | | 0.2 | | | | 0.31 | | | | | | | | | | -0.I3 | | | | | -0.16 | | | | | 0.15 |
| PSI- BLAST | | 3.60E-11 | | | | 1.80E-35 | | • | | 9.00E-38 | | | | 00 2000 | 1.20E-38 | | | | | 7.20E-38 | | | | | 1.30E-28 | | | | | 5.40E-31 |
| End | | 377 | | | | 498 | | | | 999 | | | | 17.0 | ₹ . | | | | | 754 | _ | | | | 433 | | | | | 46] |
| Start AA | | 292 | | | | 353 | | | | 521 | | | | 763 | 0/0 | | | | | 909 | | | | | 332 | | | | | 355 |
| Chain 19 | | ¥ | | _ | | ٧ | | | | A | | | | | < | | | | | ∢ | | | | | o | | | | | ပ |
| සු ස | | <u> </u> | | | | 91 | | | | 146 | | | | 37. | 8 | | | | | # | | | | | Jubd | | | | | lubd |
| ğ a Ş | | 800 | | | | 008 | | | | <u>8</u> | | _ | | 000 | 8 | | | | | 8 | _ | | _ | | 08 | | | | | 80 |

| PDB annotation | REGULATION/DNA) YING-YANG I; TRANSCRIPTION INTIATION, INTIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DA) | COMPLEX (TRANSCRIPTION REQUILATIONDNA), YNG-YRAIG I; TRANSCRIPTION INITIATION, INITIATIOR ELEMENT, YYI, 2002 FINGER PROTEIN, DINA-PROTEIN RECOGNITION, IS OMPLEX RECOGNITION, IS OMPLEX | COMPLEX (TRANSCRIPTION REQUILT/DIONDAN YING-YANG I; TRANSCRIPTION INTATION, INTIATOR ELEMBAT, YYI, 2002 FINGER PROTEIN, DINA-PROTEIN RECOGNITION, I COMPLEX (TRANSCRIPTION REGULATIONIDNA) | COMPLEX (TRANSCRIPTION REQUILATIONONA) TRANSCRIPTION INITIATION, INITIATIOS BLEMBAT, YYI, 2002 FINGER PROTEIN DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REQUIATIONDNA) YING-YANG I; TRANSCRIPTION INTIATION, INTIATION B. ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECORDITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REQUILATIONDNA) YING-YANG I; TRANSCRIPTION INTIATION, INTIATION B. ELEMENT, YYI, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX |
|----------------|---|---|--|--|---|---|
| Coumpound | ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; |
| SeqFold | | | | | | |
| PMF | | _ | - | - | 96.0 | 0.93 |
| Verify | | 0.05 | 0.51 | 0.1 | 0.12 | 0.33 |
| PSI- BLAST | | 1.30E-45 | 1.30E-57 | 7.80E-55 | 1.30E-53 | 9.00E-35 |
| End | | 461 | 489 | 245 | 109 | 629 |
| Start | | 357 | 385 | 434 | 490 | 228 |
| Chain D | | U | ပ | ပ | ပ | ပ |
| PDB DD | | Inpq | Iubd | lubd | Iubd | Iubd |
| S a S | | 008 | 800 | 008 | 008 | 008 |

| PDB annotation | COMPLEX (TRANSCREPTION REGULATIONDNA) YING-YANG I; TRANSCREPTION INITIATION, INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEN, DNA-PROTEIN RECOGNITION, SOMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REQUILATIONDNA), YING-YANG I; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YYI, ZINC 2 FINGER SPOTEIN, DIAA-PROTEIN RECOGNITION, I COMPLEX (TRANSCRIPTION REQUILATIONDNA) | COMPLEX (TRANSCRIPTION REGULATIONONA, 97 NG-YANG I; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULATIONNON, 97 YIG-Y-ANG I; TRANSCRIPTION INTITATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DIA-PROTEIN RECOGNITION, I COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULATIONNON, STGE-YANG I; TRANSCRIPTION INTIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER ROCTEN, DIAA-PROTEIN RECOGNITION, 3 COMPLEX TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YN TRO-YANG I; TRANSCRIPTION INTIA/TION, INTIA/TION, INTIA/TION, FINGER PROFIEN, DIVA-PROTEIN RECOGNITION, 3 COMPLEX |
|------------------|---|--|--|---|--|---|
| Coumpound | YYI; CHAIN: C, ADENO- SSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B. | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIANE ELMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADBNO- SASCIA/TED VIRUS PS INITIA/TOR ELMENT DIM; ÇHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; |
| SeqFold score | | 91.29 | | | | |
| PMF | - | | _ | 0.99 | - | - |
| Verify score | 0.11 | | 0.22 | 0.25 | 0.13 | 0.15 |
| PSI- BLAST | 1.30E-58 | 5.20E-60 | 3.60E-35 | 5.20E-60 | 1.60E-34 | 3.90E-61 |
| Pud AA | 657 | 658 | 637 | 713 | 713 | 741 |
| Start | 546 | 248 | 556 | 602 | 219 | 630 |
| Chain | U | U | U | U | ၁ | ပ |
| E CE | Inbd | pgn | pgn | Iubd | Iubd | Iubd |
| SEQ NO DE | 008 | 008 | 008 | 008 | 800 | 800 |

| PDB annotation | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTFIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTFIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTFIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTFINDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI, GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | STRUCTURAL PROTEIN TWO REPEATS OF SPECTRIN, ALPHA HELICAL LINKER REGION, 22 |
|-----------------|--------------------------------|--|--|--|--|--|--|--|--|--|---|
| Coumpound | | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DINA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ALPHA SPECTRIN; CHAIN: A, B, C, |
| SeqFold | | | 105.23 | | | | | | | | |
| PMF | | 0.93 | | 0.88 | 0.81 | _ | 6.0 | _ | | 0.98 | 0.37 |
| Verify score | | 0.44 | | 0.18 | 90:0 | 0.15 | 0.16 | 0.11 | 0.32 | 0.41 | -0.2 |
| PSI- BLAST | | 1.30E-43 | 3.90E-71 | 2.60E-70 | 3.90E-71 | 5.20E-73 | 1.30E-34 | 5.20E-79 | 5.40E-34 | 1.10E-33 | 0.0052 |
| End | | 463 | 519 | 547 | 603 | 631 | 929 | 743 | 712 | 743 | 302 |
| Start | | 367 | 380 | 381 | 408 | 464 | 528 | 576 | 584 | 612 | 16 |
| Chain | | ¥ | 4 | ¥ | V | ¥ | ¥ | ¥ | ¥ | 4 | A |
| PDB ID | | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | Icun |
| SEQ NO: | | 008 | 008 | 008 | 008 | 008 | 008 | 800 | 008 | 008 | 804 |

| | | | | | | _ | | _ | _ | | | | | | | | | _ | _ | | | | _ | |
|------------------|--|---------------------------------|---|--|--|---|---|----------------------|------------------------------|--------------------------------|---------------------------|---|--------------------------|-----------------|-------------------------------|--|--------------------------|----------------------------|-------------------------|-------------------------------|---------------------------------|-------------------------------|---------------------------------|--|
| PDB annotation | TANDEM 3-HELIX COILED-COILS, STRUCTURAL PROTEIN | CELL ADHESION FOUR-HELIX BUNDLE | CELL ADHESION FOUR-HELIX BUNDLE | RIBOSOME TRANSLATION, RIBOSOME, HINGE VARIABILITY | CHAPERONE ARCHAEAL PROTEIN | | GROWTH FACTOR [ABU6, 20] MEGF4- 48; GROWTH FACTOR, MURINE EPIDERMAL GROWTH FACTOR, DISULFIDE 2 CONNECTIVITIES, EGF- LIXE DOMAIN, REPEAT | COMPLEX (BLOOD | COAGULATION/INHIBITOR) | HYDROLASE, SERINE PROTEINASE), | PLASMA CALCIUM BINDING, 2 | GLYCOPROTEIN, COMPLEX (BLOOD COAGULATION/INHIBITOR) | BLOOD COAGULATION BLOOD | SERINE PROTEASE | MEMBRANE PROTEIN LECTIN-LIKE, | NEUKOBIOLOGI, CELL-CELL ADHESION CELL-CELL | RECOGNITION, ALTERNATIVE | SPLICING, MEMBRANE PROTEIN | TRANSPORT PROTEIN SHBG; | STEROID TRANSPORT, LAMININ G- | ANDROGEN BINDING PROTEIN (ABP). | SEX STEROID BINDING PROTEIN 3 | HYDROL ASE/HYDROL ASE INHIBITOR | PROTEIN-PEPTIDE COMPLEX |
| Coumpound | | ALPHA-CATENIN; CHAIN: A; | ALPHA-CATENIN; CHAIN: A; BETA-CATENIN; CHAIN: B; | RIBOSOME RECYCLING FACTOR; CHAIN: A; | PREFOLDIN; CHAIN: A; PREFOLDIN; CHAIN: B; PREFOLDIN; CHAIN: C; | | EPIDERMAL GROWTH FACTOR; CHAIN: NULL; | ACTIVATED PROTEIN C; | MAT: CHAIN: C, L; D-PHE-PRO- | , contract 1, | | | FACTOR VII; CHAIN: NULL; | | NEUREXIN-I BETA; CHAIN: | A, B, C, D, E, F, G, H; | | | SEX HORMONE-BINDING | GLOBULIN; CHAIN: A; | | | DES-GLA FACTOR VIIA | (HEAVY CHAIN); CHAIN: H, I; DES-GLA FACTOR VIIA |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 1 | 1 | 90.0 | 10'0 | | 0.58 | -0.12 | | | | | 66.0 | | 4.0 | | | | 0.72 | | | | 0.05 | |
| Verify score | | 0.41 | 0.37 | -0.65 | -0.34 | | 0.39 | 0.55 | | | | | 96.0 | | 0.26 | | | | 0.46 | | | | 0.48 | |
| PSI- BLAST | | 3.90E-59 | 6.50E-70 | 0.0072 | 1.30E-06 | | 6.50E-12 | 6.50E-19 | | | | | 1.30E-11 | | 1.30E-26 | | | | 3934 2.60E-27 | | | | 3.90E-21 | |
| End | | 257 | 257 | 14 | 103 | | 3984 | 4033 | | | | | 3987 | | 3928 | | | | 3934 | | | | 4033 | |
| Start AA | | 79 | 54 | 367 | 3 | | 3949 | 3943 | | | | | 3949 | | 3771 | | | | 3773 | | | | 3944 | |
| Chain | | A | ∢ | V | Ą | | | T | | | | | | | ٧ | | | | ٧ | | | | 1 | |
| PDB CD | | ldov | ob! w | 1eh1 | 1£k | | 1a3p | lant | | | | | 1669 | | | | _ | | 142s | | | | ldva | |
| S e S | | 804 | 804 | 804 | 804 | | 808 | 808 | | | | | 808 | | 808 | | | | 808 | | | | 808 | |

| | | | 0. 4 | | | | | |
|----------------|---|--|--|--|---|--|---|--|
| PDB annotation | | HYDROLASBHYDROLASE INHIBITOR PROTEIN-PEPTIDE COMPLEX | SERNIE PROTEINASE COAGULATION PACTOR II; CEDORULATION PACTOR II; EFEDMODULIN, TN, CD14. ANTIGER, EGR-CARG SERINE PROTEINASE, EGF-LIKE DOMAINS, ANTICOMPLEX, 2 ANTIFERRINOLYTIC COMPLEX. | CELL ADHESION PROTEIN EPTHELIAL CADHERIN DOMAINS 1 AND 2, ECADHS, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAI. CADHERIN DONAINS I AND 2, ECADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN, | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADIS: CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I |
| Coumpound | (LIGHT CHAIN); CHAIN: L, M; (DPN)-PHE-ARG; CHAIN: C, D; PEPTIDE E-76; CHAIN: X, Y; | DES-GLA FACTOR VIIA HEAVY CHAND; CHAND; HAND; I, DES-GLA FACTOR VIIA (LIGHT CHAIN); CHAND; M; (PPN)-PHE-ARG; CHAN); C, D; PEPTIDE E-76; CHAIN; X, Y; | THROWBIN LIGHT CHAIN; CHAIN: A, B, C, D, THROMBIN HEAVY CHAIN; THROMBIN HEAVY CHAIN; THROMBOMODILIN; CHAIN: I, J, K, L; THROMBIN MINBITONE LGIJU-LGLY-ARM, CHAIN: E, C, H: | E-CADHERIN; CHAIN: Á, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A. B. |
| SeqFold | | | | | | | | |
| PMF | | -0.18 | 61.0- | - | 1202.08 | 6.0 | 0.82 | -1.41 |
| Verify | - | 0.25 | 90:0 | 0.26 | 0.22 | 0.45 | 0.27 | 0.1 |
| PSI- BLAST | | 1.30E-13 | 1.30E-11 | 3.60E-33 | 1.30E-32 | 3.60E-21 | 1.60E-49 | 1.30E-32 |
| End AA | | 4344 | 4336 | 1234 | 1338 | 1440 | 1547 | 1652 |
| Start | | 4263 | 4232 | 9901 | 1171 | 1279 | 1352 | 1460 |
| Chain | | -1 | | < | ∀ | ¥ | ¥ | A |
| EDB CD | | Idva | 1dx5 | legh H | 1edh | ledh | ledh | 1edh |
| SE A SE | | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

| PDB annotation | AND 2, ECADI2, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIE; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN, | CELL ADHESION PROTEIN EPITHELAL CADHERIN DOMAINS I AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN, | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN, | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADD2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIZ; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADD2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12: CADHERIN, CELL |
|-----------------|---|--|---|--|---|---|---|---|---|
| Coumpound | | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B: | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; |
| SeqFold | | | | | | | | | |
| PMF | | 96:0 | 66.0 | _ | 0 | 96:0 | 150 | 0.78 | - |
| Verify score | | 0.21 | 0.19 | 0.32 | 0 | 0.26 | 0.3 | 0.24 | 0.18 |
| PSI- BLAST | | 3.60E-33 | 1.60E-28 | 3.60E-26 | 1.60E-20 | 3.60E-29 | 1.10E-50 | 1.30E-28 | 3.60E-48 |
| End | | 1750 | 1860 | 1960 | 354 | 2062 | 2163 | 2264 | 2371 |
| Start | | 1589 | 0691 | 1800 | 182 | 1898 | 1975 | 2104 | 2178 |
| Chain | | ∀ | ¥ | ¥ | 4 | ¥ | ¥ | < | Ą |
| PDB DD | | leg h | ledh | ledh | ledh | ledh | ledh | ledh | ledh |
| SEQ BO | | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

| | | | | | _ | | | _ | | | _ | | _ | | | | _ | | | | _ | | | | _ | _ | | | _ | _ | |
|------------------|--|--|-------------------------------|---|--------------------------|----------------------------------|---------------------------|-----------------|--------------------------|----------------------------|---------------------------|-----------------|--------------------------|-------------------------------|-------------------------------|---|--------------------------|-------------------------------|-------------------------------|---------------------------|--------------------------|-------------------------------|-------------------------------|---------------------------|--------------------------|-------------------------------|-------------------------------|---------------------------|-------------------------|--------------------------------|---|
| PDB annotation | ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I | AND 2, ECADI2; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN | AND 2 ECADIS: CADHERIN DOMAINS 1 | ADHESION PROTEIN, CALCIUM | BINDING PROTEIN | CELL ADHESION PROTEIN | AND 2 ECADIS-CADHERIN CELL | ADHESION PROTEIN CALCILIM | BINDING PROTEIN | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS 1 | AND 2, ECAD12; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM RINDING PROTEIN | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS 1 | AND 2, ECAD12; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS 1 | AND 2, ECAD12; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS 1 | AND 2, ECAD12; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM | CELL ADDRESION PROTEIN | EPITHELIAL CADHERIN DOMAINS 1 | AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM |
| Coumpound | | E-CADHERIN; CHAIN: A, B; | | | E-CADHERIN; CHAIN: A, B; | | | | E-CADHERIN; CHAIN: A, B; | | | | E-CADHERIN; CHAIN: A, B; | | | | E-CADHERIN: CHAIN: A. B. | | | | E-CADHERIN: CHAIN: A. B. | | | | E-CADHERIN; CHAIN: A. B. | | | | E-CADHERIN: CHAIN: A B. | ביייין אין אין אין אין אין אין | |
| SeqFold score | | | | | | | | | | | | | | | | | 120.62 | | | | | | | | | | | | | | |
| PMF score | | 1 | | | 98.0 | | | | 0.93 | | | | 96.0 | | | | | | | | 1 | | | | _ | | | | 70 0 | 5 | |
| Verify | | 0.32 | | | 0.07 | | | | 0 | | | | 0.1 | | | | | | | | 0.47 | | | | 0.27 | | | | 0.31 | 1 | |
| PSI- BLAST | | 2473 1.60E-35 | | | 1.80E-29 | | | | 1.80E-38 | | | | 5.40E-32 | | | | 1.80E-57 | | | | 1.80E-57 | | | | 7.20E-35 | | | | 3105 5 40E-20 | | |
| End AA | | 2473 | | | 2577 | | | | 2683 | | | | 2789 | | | | 2895 | | | | 2898 | | | | 3003 | | | | 3105 | 3 | |
| Start AA | | 2306 | | | 2414 | | | | 2488 | | | | 6192 | | | | 2692 | | | | 2693 | | | | 2831 | | | | 2941 | : | |
| Chain | | ∢ | | | ۷ | | | | ∢ | | | | ¥ | | | | < | | | | V | | | | 4 | | | | 4 | : | |
| EDB ID | | ledh H | | | ledh | | | | eg- | | | | ledh | | | | Eg. | | | | legh | | | | ledh | | | | ledh | | |
| SEQ B B SE | | 808 | | | 808 | | | | 808 | | | | 808 | | | | 808 | | | | 808 | | | | 808 | | | | 808 | | |

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|-----------------|-----------------|--|--|--|---|--|--|--|---|
| PDB annotation | BINDING PROTEIN | CELL ADHESION PROTEIN EPTHELIAL CADHERIN DOMAINS I AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADI 2, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPTHELIAL CADHERIN DOMAINS I AND 2, ECADIS, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCTUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI-S, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI S. CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIS, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN |
| Coumpound | | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; |
| SeqFold | | | | | | | | | |
| PMF | | 0.53 | 0.64 | -1.41 | 0.98 | - | 0.3 | 0.83 | 0.82 |
| Verify score | | 0.38 | 0.16 | 0.57 | 0.45 | 99:0 | 0.12 | 0.29 | 0.17 |
| PSI- BLAST | | 7.20E-25 | 5.40E-28 | 1.80E-32 | 1.80E-48 | 3.60E-30 | 1.80E-51 | 1.10E-29 | 3.60E-29 |
| End | | 450 | 3197 | 3313 | 3418 | 3523 | 248 | 556 | 799 |
| Start | | | 3046 | 3120 | 3225 | 3355 | 39 | 406 | 464 |
| Chain ID | | Υ | ٧ | ¥ | A | ٧ | V | ٧ | ¥ |
| PDB ID | | ledh | 1edh | 1edh | ledh | ledh | ledh | ledh | ledh |
| SEQ NO: | | 808 | 808 | 808 | . 808 | 808 | 808 | 808 | 808 |

| PDB annotation | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BNDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD IS, CADHERIN, CELL ADHESION PROTEIN, CALCTUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | MATRIX PROTEIN EXTRACELLULAR MATRIX, CALCIUM-BINDING, GLYCOPROTEIN, 2 REPEAT, SIGNAL, MULTICENE FAMILY, DISEASE MULTICENE FAMILY, DISEASE MULTICN, 3 EGF-LIKE DOMAIN, HUMAN PIBRILLIN-I FRAGMENT, MATRIX PROTEIN | CELL ADHESION PROTEIN EGF-LIKE DOMAIN, CELL ADHESION PROTEIN, TRANSMEMBRANE, 2 GLYCOPROTEIN | GLYCOPROTEIN GLYCOPROTEIN | GLYCOPROTEIN GLYCOPROTEIN | GLYCOPROTEIN GLYCOPROTEIN CELL ADHESION PROTEIN CADHERIN | CELL ADHESION PROTEIN CADHERIN | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN |
|----------------------|---|--|--|---|---|--|---------------------------|---------------------------|--|--------------------------------|---|--------------------------------|
| Coumpound | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | FIBRILLIN; CHAIN: NULL; | P-SELECTIN; CHAIN: NULL; | LAMININ; CHAIN: NULL; | LAMININ; CHAIN: NULL; | LAMININ; CHAIN: NULL; N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 |
| SeqFold | | | | | | | | | | | | |
| PMF | 0.27 | - | - | 69.0 | 0.99 | 0.88 | 0.27 | -0.03 | 0.29 | 69.0 | 0.29 | 0.1 |
| Verify | -0.05 | 0.33 | 0.31 | 0.11 | 0.71 | 1.03 | -0.1 | 0.07 | 0.12 | 0.13 | 0.01 | 0.46 |
| PSI. BLAST | 5.40E-22 | 1.10E-55 | 1.10E-32 | 9.00E-32 | 1.80E-16 | 1.30E-11 | 1.10E-13 | 5.40E-21 | 3.60E-17 9.00E-06 | 0.00014 | 1.40E-14 | 1546 0.00018 |
| End | 812 | 716 | 1022 | 1129 | 4022 | 3988 | 4050 | 4075 | 1127 | 1232 | 1439 | 1546 |
| Start | 165 | 718 | 854 | 959 | 3946 | 3949 | 3924 | 3954 | 1062 | 1167 | 1350 | 1480 |
| Chain | ∢ | V | ٧ | ∢ | | | | | | | | |
| EDB CI | 1edh | ledh | ledh | ledh | lem n | 1£\$ | Iklo | k k | Incg | Incg | Incg | Incg |
| SE Se Se Se | 808 | 808 | 808 | 808 | 808 | 808 | 8 | 808 | 808 | 808 | 808 | 808 |

| | Γ | ERIN | ERIN | ERIN | ERIN | ERIN | ERIN | ERIN | ERIN | ERIN | ERIN | ERIN | ERIN |
|------------------|--------|---|---|---|---|---|---|---|---|---|--------------------------------|---|---|---|---|--|---|---|---|---|--------------------------------|
| e e | | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN |
| PDB annotation | | PROTE | PROTE | PROTE | I PROTEI | PROTE | PROTE | PROTE | PROTE | PROTE | PROTE | PROTE | PROTE | PROTE | PROTE | PROTE | I PROTE | PROTE | PROTE | PROTE | PROTE |
| PDB | _ | DHESION | DHESION | DHESION | DHESION | DHESTON | DHESION | OHESION 3 | DHESION | DHESION | DHESTON | DHESION | DHESION | DHESION | DHESTON 3 | DHESION | DHESTON | DHESION | DHESTON | DHESTON | DHESION |
| | INGG I | CELL AD | CELL AD | CELL AD | CELL AD | CELL AD INCG 13 | CELL AD | CELL AD INCG 13 | CELL AD | CELL AD INCG 13 | CELL AD | CELL AD INCG 13 | CELL AD | CELL AD INCG 13 | CELL AD INCG 13 | CELL AD INCG 13 | CELL AD | CELL AD | CELL A | CELL AI | CELLA |
| | | | | | | | | | | | | | | | | | | | | | |
| Coumpound | | ; INCG 3 | , INCG 3 | 1NCG 3 | 1NCG3 | INCG 3 | : INCG 3 | : INCG 3 | , INCG 3 | 1NCG3 | , INCG 3 | ; INCG 3 | , INCG 3 | ; INCG 3 | ; INCG 3 | ; INCG 3 | ; INCG 3 | , INCG 3 | ; INCI 3 | ; INCI 3 | INCI 3 |
| Coun | | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; 1NCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 |
| | L | Y-CA | A CA | N-CA | N-CA | A-CA | N-CA | A CA | Y V | N-CA | N-CA | S S | N-CA | N-CA | NCA | S CA | S CA | S N | NCA | N.C. | NCA |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 60:0 | 60.0 | 0.31 | 0.1 | 0.11 | 0.1 | 0.74 | 0.43 | 0.57 | 0.7 | 0.39 | 0.51 | 0.34 | 0.36 | 8.0 | 0.53 | 0.64 | 0.78 | 96.0 | 0.22 |
| Verify score | | 0.15 | -0.13 | 0.35 | 0.22 | 0.28 | -0.08 | 0.41 | -0.27 | 0.34 | 0.44 | 0.35 | 0.45 | 90.0 | 0.33 | 91.0 | -0.19 | 0.38 | 90:0 | 90.0 | 0.43 |
| PSI- BLAST | | 3.60E-05 | 9.00E-06 | 3.60E-06 | 3.60E-17 | 0.00036 | 3.60E-12 | 1.80E-06 | 0.00036 | 1.60E-05 | 1.80E-19 | 0.00054 | 3.60E-06 | 1.80E-05 | 1.60E-11 | 7.20E-20 | 0.00018 | 5.40E-05 | 1.80E-06 | 5.40E-05 | 1.30E-13 |
| End | | 525 | 1650 | 1748 | 2061 | 2161 | 2263 | 2370 | 2458 | 2681 | 2788 | 2988 | 3106 | 3191 | 3311 | 811 | 006 | 1003 | 1129 | 1234 | 1440 |
| Start AA | | 155 | 1599 | 1667 | 1970 | 2079 | 2178 | 2304 | 2411 | 2593 | 2692 | 2913 | 3039 | 3120 | 3225 | 91,6 | 852 | 932 | 1065 | 1172 | 1350 |
| Chain | | | | | | | | | | | | | | | | | | | В | м | Д |
| 808 E1 | | Incg | Incg | Incg | Incg | Incg | Incg | lncg | Incg | Incg | Incg | Incg | lncg | lncg | Incg | lncg | Incg | lncg | Inci | lnci | Inci |
| S a S | | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

| PDB annotation | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL |
|------------------|---|---|--------------------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|--------------------------------|---|---|---|----------------------------|
| Coumpound | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | |
| PMF | 9.65 | 9.0 | 0.4 | 0.23 | 0.05 | 0.1 | 0.75 | 0.58 | 90.0 | ı. | 0.92 | 0.42 | 0.17 | 0.49 | 66'0 | 96'0 | 0.71 | 0.63 | _ | _ | 0.54 |
| Verify score | -0.08 | 0.35 | -0.17 | 0.08 | -0.25 | -0.11 | 0.17 | -0.14 | 0 | 0.56 | 0.42 | 0.56 | -0.2 | 0.67 | 0.87 | 0.15 | -0.4 | 0.36 | 0.45 | 0.34 | 0.3 |
| PSI- BLAST | 0.00018 | 9.00E-07 | 1.60E-05 | 1.80E-16 | 0.0013 | 1,30E-11 | 5.40E-07 | 60000 | 1.60E-05 | 3.60E-19 | 0.0036 | 5.40E-06 | 0.00036 | 1.80E-10 | 1.80E-08 | 1.80E-19 | 5.40E-05 | 1.80E-05 | 3.60E-36 | 5.40E-33 | 1.80E-22 |
| End | 1547 | 1750 | 248 | 2062 | 2163 | 2264 | 2371 | 2458 | 2683 | 2789 | 3003 | 3105 | 3191 | 3313 | 3418 | 812 | 116 | 1022 | 1234 | 1338 | 1440 |
| Start AA | 1491 | 1991 | 181 | 1970 | 2116 | 2178 | 2307 | 2414 | 2620 | 7692 | 2942 | 3044 | 3146 | 3225 | 3354 | 715 | 862 | 932 | 1039 | 1147 | 1270 |
| Chain D | В | В | В | В | Я | В | В | В | В | В | В | В | В | В | В | В | В | В | ٧ | A | ٧ |
| PDB CI | Inci | lnci. | Inci | Inci | Inci | lnci | Inci | Inci | lnci | Inci | luci . | Inci | lnci | Inci | Inci | Inci | Inci | lnci | Incj | Incj | Inci |
| S e S | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 88 | 808 | 808 | 808 | 808 | 88 |

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CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL ADHESION PROTEIN CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL CELL ADHESION PROTEIN CELL PDB annotation ADHESION PROTEIN N-CADHERIN, CHAIN: A: N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN: CHAIN: A: N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; N-CADHERIN; CHAIN: A; SeqFold score 20.25 core PMF 0.58 96.0 0.76 0.33 98.0 0.83 6.0 3 Verify Score -0.05 -0.03 0.29 0.62 0.03 0.05 0.45 0.31 0.42 5 0.48 0.17 0.27 0.14 0.25 0.28 0.31 9 1.30E-32 1.40E-31 BLAST 3.60E-32 7.20E-55 5.40E-52 5.40E-36 7.20E-32 1.60E-41 5.40E-63 3.60E-38 1.80E-29 3.60E-53 1.80E-34 5.40E-24 3.60E-33 7.20E-27 3.60E-28 3.60E-30 3.60E-27 5.40E-63 3003 3196 1547 1652 1750 1981 1960 2062 2163 2264 2371 2577 2683 2789 2897 2898 3105 ₽ ¥ 2473 55 354 Start 1458 1667 2079 2178 2300 2488 2593 2693 2825 2913 3039 1351 1898 1970 2407 2691 55 256 Chain 19 ¥ ⋖ 4 4 4 ¥ ⋖ ¥ ⋖ ⋖ 4 ⋖ ⋖ ⋖ ⋖ **B** 10. 5 5 lo: 5 5 ing a lo: 2 5 Inc. 딛 . C 5 lici ë 800 808 88 808 808 808 808 808 8 8 808 8 8 808 808 8 808 88 808 808

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|------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|-------------------------------|---|---------------------|----------------------|---|-----------------------|-----------------------|
| PDB annotation | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | COMPLEX (BLOOD COAGULATION/INHIBITOR) CHRUSTMAS FACTOR; COMPLEX, INHIBITOR HEMOPHILIAFICE | BLOOD COAGULATION, 2 PLASMA, BLOOD COAGULATION, 2 PLASMA, BRING PROTEASE, CALCIUM- BINDING, HYDROLASE, 3 GLYCOPROTEIN | SERINE PROTEASE FVIIA; FVIIA; | BLOOD COAGULATION, SERINE PROTEASE | | | SERINE PROTEASE FVIIA; BLOOD COAGULATION, SERINE | PROTEASE | |
| Coumpound | N-CADHERIN; CHAIN: A; | FACTOR IXA; CHAIN: C, L,; D-PHE-PRO-ARG; CHAIN: I; | *1 | COAGULATION FACTOR | VIIA (LIGHT CHAIN); CHAIN: L; COAGULATION FACTOR | VIIA (HEAVY CHAIN); | INHIBITOR; CHAIN: C; | COAGULATION FACTOR VIIA (LIGHT CHAIN); CHAIN: | L; COAGULATION FACTOR | CHAIN: H; TRIPEPTIDYL |
| SeqFold score | | | | | | | | | | | | | | | | | | | | |
| PMF | 9.63 | 66.0 | 1 | 0.39 | 0.21 | 0.35 | 66.0 | 0.18 | _ | 0.88 | - | -0.19 | | -0.19 | | | | 25.0 | | |
| Verify score | 0.36 | 0.48 | 0.63 | 0.52 | -0.28 | 0.3 | 0.37 | 0.02 | 0.23 | 0.34 | 0.39 | 0.01 | | 0.2 | | | | 89.0 | | |
| PSI- BLAST | 1.80E-34 | 7.20E-51 | 3.60E-32 | 3.60E-13 | 1.80E-57 | 1.80E-34 | 9.00E-30 | 1.80E-25 | 7.20E-62 | 1.80E-34 | 1.10E-34 | 1.40E-10 | | 1.30E-11 | | | | 1.20E-21 | | |
| End | 3313 | 3418 | 3523 | 3621 | 248 | 929 | 299 | 812 | 917 | 1022 | 1129 | 4312 | | 4001 | | | | 4033 | | |
| Start AA | 3120 | 3225 | 3346 | 3433 | 39 | 390 | 494 | 172 | 717 | 827 | 932 | 4224 | | 3943 | | | | 1568 | | |
| Chain ID | ¥ | A | A | V | ٧ | ٧ | ¥ | ٧ | ٧ | ٧ | Ą | 7 | | 7 | | | | ۔۔۔ | | |
| PDB DD | Incj | lncj | Incj | lncj | Incj | Incj | Incj | Incj | Incj | lncj | lnej | 1pfx | | 1qfk | | | | Iqfk | | |
| SEQ No. 10 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | | 808 | | | | 808 | | |

| PDB annotation | | SERINE PROTEASE PVILA; PVIIA; BLOOD COAGULATION, SERINE PROTEASE | SERINE PROTEASE FYIIA; FYIIA; BLOOD COAGULATION, SERINE PROTEASE | COAGULATION FACTOR SERINE PROTEINASE, BLOOD COAGULATION, COAGULATION FACTOR | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION |
|----------------|----------------------|--|---|---|--|--|--|--|--|--|--|--|
| Coumpound | INHIBITOR; CHAIN: C; | COAGULATION FACTOR VIA (LIGHT CHAIN); CHAIN; L; COAGULATION FACTOR VIIA (HEAVY CHAIN); CHAIN: H; TRIPEPTIDYL INHIBITOR: CHAIN: C | COAGULATION FACTOR VIIA (LIGHT CHAIN); CHAIN; L; COAGULATION FACTOR VIIA (HEAVY CHAIN); CHAIN: H; TRIPEPTIDYL INHIBITOR; CHAIN: C | COAGULATION FACTOR IX; CHAIN: A; COAGULATION FACTOR IX; CHAIN: B; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; |
| SeqFold | | | | | | | | | | | | |
| PMF | | -0.17 | -0.17 | -0.19 | 0.27 | 0.93 | 0.45 | 0.62 | 0.13 | 0.04 | 0.63 | 0.07 |
| Verify | | 0 | 0.37 | 0.03 | 0.24 | 90:0- | 0.04 | 0.54 | 0.28 | 0.37 | 0.45 | 0.35 |
| PSI- BLAST | | 5.40E-14 | 7.20E-13 | 7.80E-14 | 7.80E-20 | 1.60E-07 | 1.30E-17 | 1.30E-10 | 0.0013 | 1.80E-19 | 1.30E-08 | 2.60E-07 |
| End AA | | 4202 | 4344 | 4001 | 1133 | 1133 | 1238 | 1334 | 1342 | 1444 | 1549 | 226 |
| Start | | 4121 | 4267 | 3951 | 1041 | 1066 | 1145 | 1249 | 6/21 | 1350 | 1455 | 155 |
| Chain | | J | ı. | ш. | | | | | | | | |
| PDB ID | | 1qfk | 1 _q fk | 恒 | 1suh | 1suh | Isuh | 1suh | 1suh | 1suh | Isuh | lsuh |
| SEQ No. | | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

| PDB annotation | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN. CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN: CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL |
|------------------|--|--|--|--|--|--|--|--|--|--|--|--|--|--|
| Coumpound | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; |
| SeqFold score | | | | | | | | | | | | | | |
| PMF | 0.31 | 0.13 | 89.0 | 0.75 | 0.48 | 0.45 | 0.13 | 60:0 | 0.4 | 0.77 | 0.94 | 0.58 | 0.25 | 0.15 |
| Verify score | 0.41 | -0.2 | 0.07 | 0.17 | -0.06 | -0.18 | -0.41 | 0.42 | -0.37 | 0.44 | 0.35 | 0.03 | -0.04 | -0.37 |
| PSI- BLAST | 1.00E-12 | 9.00E-09 | 1.30E-12 | 3.60E-06 | 1.30E-14 | 3.60E-05 | 1.80E-06 | 2.60E-15 | 1.30E-15 | 3.90E-20 | 2375 3.60E-09 | 3.90E-05 | 3.60E-05 | 1.80E-12 |
| End | 1650 | 1656 | 1754 | 1754 | 1867 | 1868 | 252 | 2163 | 2268 | 2375 | 2375 | 2475 | 2477 | 2581 |
| Start AA | 1570 | 1589 | 1991 | 0691 | 1771 | 1800 | 182 | 2084 | 2178 | 2280 | 2306 | 2395 | 2414 | 2488 |
| Chain ID | | | | | | | | | | | | | | |
| 708 CD | lsuh | 1suh | 1suh | 1suh | Isuh | lsuh | Isuh | Isuh | 1suh | Isuh | Isuh | Isuh | 1suh | Isuh |
| ğa ÿ | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

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|------------------|----------|--|--|--|--|--|--|--|--|--|--|--|--|--|---------------------------|
| PDB annotation | ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCTUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCTUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; |
| Coumpound | | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; |
| SeqFold score | | | | | | | | | | | | | | | ٨ |
| PMF | | 0.98 | 0.12 | 66:0 | 0.87 | 0.25 | 0.93 | 0.86 | 0.89 | 0.72 | 0.28 | 0.25 | 0.82 | 86.0 | 0.93 |
| Verify | | 0.16 | 0.02 | 0.42 | 0.43 | 0.01 | 0.37 | -0.07 | 0.36 | 0.4 | 0.1 | 0.43 | 9.0 | 0.58 | 99.0 |
| PSI- BLAST | | 1.30E-13 | 2.60E-10 | 3.60E-23 | 2.60E-21 | 3.60E-09 | 1.20E-14 | 1.80E-06 | 2.60E-21 | 3109 3.60E-06 | 0.0013 | 3213 3.90E-12 | 1.10E-14 | 3.90E-21 | 1.30E-09 |
| End AA | | 2581 | 2681 | 2793 | 2902 | 2902 | 3007 | 3007 | 3109 | 3109 | 3185 | 3213 | 3317 | 3422 | 3422 |
| Start AA | | 2489 | 2591 | 2692 | 2806 | 2831 | 2914 | 2941 | 3026 | 3046 | 3120 | 3120 | 3225 | 3330 | 3355 |
| Chain ID | | | | | | | | | | | | | | | |
| PDB ID | | Isuh | Isuh | 1suh | 1suh | Isuh | 1suh | Isuh | 1suh | lsuh | lsuh | 1suh | 1suh | 1suh | Isuh |
| SEQ NO: | | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

| PDB annotation | CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | PLASMINOGEN ACTIVATION | BLOOD COAGULATION FACTOR STUART FACTOR, BLOOD COAGULATION FACTOR, SERINE PROTEINASE, EPIDERMAL 2 GROWTH FACTOR LIKE DOMAIN | | COMPLEX (BLOOD |
|-----------------|--|--|--|--|--|--|---|--|---|--|--|--|--|----------------------|
| Coumpound | CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | T-PLASMINOGEN ACTIVATOR F1-G; 1TPG 7 CHAIN: NULL; 1TPG 8 | BLOOD COAGULATION FACTOR XA; CHAIN: L, C; | LECTIN (AGGLUTININ) WHEAT GERM AGGLUTININ (ISOLECTIN 2) 9WGA 3 | ACTIVATED PROTEIN C; |
| SeqFold | | | | | | | | | | | | | | |
| PMF | | 0.65 | 0.24 | 61.0 | 0.19 | 0.57 | 0.95 | 0.72 | 0.45 | 0.57 | 0.59 | -0.19 | -0.2 | -0.12 |
| Verify score | | 0.56 | 80.0 | -0.6 | -0.03 | 0.39 | -0.21 | 0.4 | 0.17 | 0.37 | 0.21 | 0.15 | 0.05 | 0.55 |
| PSI- BLAST | | 6.50E-11 | 0.0001 | 1.60E-05 | 1.30E-15 | 3.90E-05 | 1.40E-23 | 1.00E-17 | 5.40E-07 | 5.20E-13 | 1.30E-18 | 5.40E-12 | 4337 3.60E-10 | 6.50E-19 |
| End AA | | 3524 | 454 | 454 | 995 | 859 | 918 | 921 | 921 | 1026 | 4026 | 4348 | 4337 | 3947 |
| Start AA | | 3435 | 363 | 406 | 467 | 290 | 116 | 826 | 854 | 930 | 3949 | 4267 | 4166 | 3857 |
| Chain ID | | | | | | | | | | | | 7 | ٧ | -1 |
| PDB D | | Isuh | 1suh | Isuh | lsuh | 1suh | Isuh | 1suh | Isuh | lsuh | ltpg | 1xka | 9wga | lant |
| SEQ NO: | | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

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|------------------|--|---|--|--|--|---|
| PDB annotation | COAGULATIONINHIBITOR) AUTOPROTRROMBIN III, HYDROLAES, SERNE PROTEINASE), PLASMA CALCIUM BINDING, 2 GLYCOPROTEIN, COMPLEX (BLOOD COAGULATIONINHIBITOR). | BLOOD COAGULATION, SERNE PROTEASE, COMPLEX, COFACTOR, 2 EEGEPTOR ENZYME, INHBITOR, GLA, EGF, 3 COMPLEX (SERNE PROTEASE/COFACTOR/LIGAND) | BLOOD COAGULATION, SERINE PROTEASE, COMPLEX, COFACTOR, 2 RECEPTOR ENZYMG, INHBITOR, GLA, EGF, 3 COMPLEX (SRENE PROTEASE/COFACTOR/LIGAND) | HYDROLASGHYDROLASE INHIBITOR PROTEIN-PEPTIDE COMPLEX | HYDROLASE/HYDROLASE INHIBITOR PROTEIN-PEPTIDE COMPLEX | HYDROLASEHYDRÖLASE INHIBITOR PROTEIN-PEPTIDE COMPLEX |
| Coumpound | CHAIN: C, L; D-PHE-PRO- MAI; CHAIN: P; | BLOOD COAGULATION FACTOR VIIA, CARNIL, H; SOLUBLE TISSUE RACTOR; CHAIN: 1, U. D-PHE-PHE- ARG. CHLOROMETHYLKETONE CHLOROMETHYLKETONE OPFROMM) WITH CHAIN: C. | BLOOD COAGULATION PACTOR VILLA, CHARIL, H. SOLJBLE TISSUE PACTOR; CHAIN! T, U, D-PHE-PHB- ARG- CHOROMETHYLKETONE CHOROMETHYLKETONE OPPROAM) WITH CHARIC. | DES-GLA FACTOR VIIA (HEAVY CHANI); CHANI; H, I; DES-GLA FACTOR VIIA (LIGHT CHAIN); CHAIN; L, M; (DPN)-PHE-ARG; CHAIN; C, D; PEPTIDE E-76; CHAIN; X, Y; | DES-GLA FACTOR VIIA (ELRAY V CHANI); CHANI: H, (ELGHT CHANI); CHANI: H, M; (DPN)-PHE-ARG; CHANI: X, Y; | DES-GLA FACTOR VIIA (ERLAY CHAND); CHAIN: H, I; DES-GLA FACTOR VIIA (LIGHT CHAIN); CHAIN: L, M; (PPI)-PHE-ARG; CHAIN: C, D; PEPTIDE E-76; CHAIN: X, Y; |
| SeqFold score | | | | | | |
| PMF | | 0.07 | 0.07 | 0.15 | 0.05 | -0.07 |
| Verify score | | 60.0 | 0.1 | -0.08 | 0.48 | 0.12 |
| PSI- BLAST | | 1.40E-12 | 3.60E-14 | 1.40E-12 | 3.90E-21 | 3.60E-14 |
| End | | 3897 | 3976 | 3897 | 3947 | 3976 |
| Start AA | | 3831 | 3900 | 3831 | 3858 | 3900 |
| Chain | | J | ī | ı | ı | _ |
| PDB ID | | 1dan | 1dan | ldva | Idva | 1dva |
| SEQ NO EI | | 808 | 808 | 808 | 808 | 808 |

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|-----------------|---|--|---|---|---|---|---|---|
| PDB annotation | HYDROLASEHYDROLASE INHIBITOR PROTEIN-PEPTIDE COMPLEX | HYDROLASE/HYDROLASE INHIBITOR PROTEIN-PEPTIDE COMPLEX | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND S, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND S, EGAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADHS, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 |
| Coumpound | DES-GLA FACTOR VIIA HEAVY CHAND; CHAND: H, I; DES-GLA FACTOR VIIA (LIGHT CHAND; CHAND: L, M; (DPN)-PHE-ARC; CHAND: C, P, PEPTIDE E-76; CHAND: X, Y; | DES-GLA FACTOR VIIA HERVY CHAIN; CHAIN: H. i: DES-GLA FACTOR VIIA GLIGHT CHAIN; CHAIN: L. M; (DPN)-PHE-ARC; CHAIN: X, Y; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; |
| SeqFold | | | | | | | | |
| PMF | -0.15 | -0.19 | _ | 96'0 | 0.93 | 0.89 | 0.65 | -1.41 |
| Verify score | 0.05 | 0.25 | 0.35 | 0.16 | 0.23 | 0.3 | 0.03 | 0.19 |
| PSI- BLAST | 3.60E-12 | 1.30E-13 | 1.10E-33 | 9.00E-30 | 1.60E-20 | 3.60E-54 | 7.20E-32 | 3.60E-33 |
| End | 4168 | 4259 | 1234 | 1338 | 1440 | 1547 | 1652 | 1750 |
| Start AA | 4078 | 4170 | 1026 | 1171 | 1279 | 1352 | 1455 | 1589 |
| Chain D | ı | J. | ٧ | ¥ | ٧ | Ą | ¥ | ٧ |
| සු ය | Idva | Idva | ledh | ledh | 1edh | 1edh | ledh | ledh |
| Še Š | 808 | 808 | 808 | 808 | | 808 | 808 | 808 |

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| PDB annotation | AND 2, ECADI 2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2. ECADIS; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BININNI PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2. ECAD12: CADHERIN CFLI. |
| Coumpound | | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; |
| SeqFold | | | | | | | | | |
| PMF | | 0.25 | 66.0 | 0.07 | 0.94 | 0.34 | 0.92 | _ | -1.41 |
| Verify | | -0.18 | 0.21 | 0.17 | 0.3 | 0.13 | 0.19 | 80:0 | 0.37 |
| PSI- BLAST | | 3.60E-28 | 1.80E-27 | 5.40E-20 | 1.80E-30 | 1.80E-50 | 9.00E-29 | 1.80E-38 | 1.80E-32 |
| End | | 1860 | 1960 | 354 | 2062 | 2163 | 2264 | 2371 | 2473 |
| Start AA | | 1690 | 1780 | 182 | 1898 | | 2104 | 2178 | 2306 |
| Chain ID | | ¥ | ∢ | 4 | ¥ | ٧ | ٧ | < . | ¥ |
| PDB CD | | ledh | ledh |
| SEQ NO: | | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

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|----------------|--|---|-------------------------------|--|--------------------------|--|--|--------------------------|----------------------------|--------------------------|-----------------|--------------------------|-------------------------------|-------------------------------|-----------------|--------------------------|-------------------------------|-------------------------------|---|--------------------------|-------------------------------|-------------------------------|-----------------|--------------------------|-------------------------------|-------------------------------|---------------------------|--------------------------|-------------------------------|---|
| PDB annotation | ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 | AND 2, ECAD12; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS I AND 2 FCAD12: CADHERIN CELL | ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN | AND 2 ECADIS: CADRERN CELL | ADHESION PROTEIN CALCUIM | BINDING PROTEIN | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS 1 | AND 4, ECADIZ; CADHERIN, CELL | BINDING PROTEIN | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS 1 | AND 2, ECAD12; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS I | AND 2, ECADI2; CADHERIN, CELL | BINDING PROTEIN | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS 1 | AND 2, ECADIZ; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS I | AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN CALCITIM |
| Coumpound | | E-CADHERIN; CHAIN: A, B; | | | E-CADHERIN; CHAIN: A, B; | | | E-CADHERIN; CHAIN: A, B; | | | | E-CADHERIN; CHAIN: A, B; | | | | E-CADHERIN; CHAIN: A, B; | | | | E-CADHERIN; CHAIN: A, B; | | | | E-CADHERIN; CHAIN: A, B; | | | | E-CADHERIN: CHAIN: A. B. | | |
| SeqFold | | | | | | | | | | | | 120.62 | | | | | | | | | | | | | | | | | | |
| PMF score | | 98'0 | | | 0.75 | | | 66.0 | | | | | | | | - | | | | | 1202.08 | | | 0.94 | | | | 0.41 | | |
| Verify | | 0.07 | | | 0.14 | | | 0.33 | | | | | | | | 0.52 | | | | 0.46 | | | | 0.31 | | | | 0.15 | | |
| PSI- BLAST | | 3.60E-29 | | | 1.60E-39 | | | 7.20E-31 | | | | 5.40E-58 | | | | 5.40E-58 | | | | 1.80E-33 | | | | 1.80E-28 | | | | 5.40E-24 | | |
| End | | 2577 | | | 2683 | | | 2789 | | | | 2895 | | | | 2898 | | | | 3003 | | | | 3105 | | | | 659 | | |
| Start AA | | 2414 | | | 2488 | | | 2619 | | | | 2692 | | | | 2693 | | | | 2831 | | | | 2941 | | | | 296 | | |
| Chain D | | ∢ | | | V | | | ٧ | | | | ¥ | | | | 4 | | | | ¥ | | | | A | | | | Ą | | |
| PDB ID | | 뜅 | | | ledh | | | 1edh | | | | ledh | | | | g | | | | ledi | | | | ledh | | | | ledh | | |
| SEQ NO ID | | 808 | | | 808 | | | 808 | | | | 808 | | | | 808 | | | | 808 | | | | 808 | | | | 808 | | |

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|-----------------|-----------------|---|--|--|--|---|--|---|---|
| PDB annotation | BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIE, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI-S, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD 12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL. CADHERIN DOMAINS I AND 2, ECADI 2, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN PPITHELIAL CADHERIN DOMAINS I AND 2, ECADHS, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN |
| Coumpound | | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: Á, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; |
| SeqFold | | | | | | | | 7 | |
| PMF | | 9.0 | 0.59 | 860 | _ | 0.3 | 0.89 | 0.77 | - |
| Verify score | | 0.28 | 0.15 | 0.53 | 0.47 | 0.12 | 0.31 | 0.5 | 0.33 |
| PSI- BLAST | | 1.80E-27 | 1.80E-28 | 1.40E-35 | 1.80E-16 | 3.60E-53 | 5.40E-30 | 3.60E-27 | 1.10E-57 |
| End AA | | 1618 | 3313 | 3418 | 3523 | 248 | 556 | 799 | 917 |
| Start | | 3045 | 3147 | 3225 | 3355 | 36 | 401 | 465 | 718 |
| Chain | | ¥ | ¥ | Ą | ¥ | ¥ | ٧ | ∢ | A |
| 708 ID | | ledh | ledh | ledh | ledh | ledh | ledh | ledh | ledh |
| S e S | | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

| PDB annotation | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADHS: CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | MATRIX PROTEIN EXTRACELLULAR MATRIX, CALCIUM-BINDING, GLYCOPROTEIN, 2 REPEAT, SIGNAL, MULTIGENE PAMILY, DISEASE MUTATION, 3 EGF-LIKE DOMAIN, HUMAN FIBRILLIN-I FRAGMENT, | MATRIX PROTEIN EXTRACELLULAR MATRIX, CALCUIM-BINDING, GLYCOPROTEIN, 2 REPET, SIGNAL, MULTIGENE FAMILY, DISEASE MUTATION, 3 EGF-LIKE DOMAIN, HUMAN FIBRILLIN-I FRAGMENT, | BLOOD CLOTTING COMPLEX(SERNE PROTEASEOVA-CHORLIGAND), BLOOD COAGULATION, 2 SERNE PROTEASE, COMPLEX, CO-PA-CTOR, GEGETOR ENZYME, 3 INHIBITOR, GLA, EGF, COMPLEX (SERNE 4 PROTEASE/CORPACTOR/LIGAND), BI ODD CLOTTING | BLOOD CLOTTING COMPLEX(SERNE PROTRASPCORACIONALIO, M.) BLOOD COAGULATION, 2 SERNE PROTRASE, COMPLEX, CO-FACTOR, RECEPTOR RAZYMS, 3 INHEBTOR, GLA, EGF, COMPLEX (SERNE 4 PROTRASE/CORACIONALIGAND), | GLYCOPROTEIN GLYCOPROTEIN |
|----------------|---|---|---|--|--|---|---------------------------|
| Coumpound | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | FIBRILLIN; CHAIN: NULL; | FIBRILLIN; CHAIN: NULL; | BLOOD COAGULATION FACTOR VIIA; CHAIN: L; BLOOD COAGULATION FACTOR VIIA; CHAIN: H; SOLUBLE TISSUE FACTOR; CHAIN: T; 5LJ5; CHAIN: I; | BLOOD COAGULATION FACTOR VILA; CHAIN: L; BLOOD COAGULATION FACTOR VILA; CHAIN: H; SOLUBLE TISSUE PACTOR; CHAIN: T; 5L15; CHAIN: I; | LAMININ; CHAIN: NULL; |
| SeqFold | | | | | | | |
| PMF | - | 0.52 | 0.48 | -0.18 | -0.01 | -0.19 | -0.2 |
| Verify | 0.14 | 0.24 | 90.0 | 0.02 | 0.12 | 0.2 | 0.07 |
| PSI- BLAST | 1.80E-33 | 1.80E-30 | 3.60E-16 | 9.00E-14 | 3.60E-14 | 1.30E-13 | 4228 1.80E-17 |
| End | 1022 | 1129 | 3931 | 4217 | 3976 | 4259 | 4228 |
| Start | 854 | 959 | 3860 | 4126 | 3900 | 4170 | 4074 |
| Chain TO | ٧ | ¥ | | | <u></u> | <u>,</u> | |
| PDB DD | ledh | ledh | lem n | lem n | Tax | Ifak | Iklo |
| SEQ NO: | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

| PDB annotation | GLYCOPROTEIN GLYCOPROTEIN | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 |
|----------------|---------------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Coumpound | LAMININ; CHAIN: NULL; | N-CADHERIN; 1NCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; 1NCG 3 | N-CADHERIN; INCG 3 |
| SeqFold | | | | | | | | | | | | | | | | | | | | | |
| PMF | -0.2 | 0.63 | 0.87 | 0.3 | 0.72 | 60:0 | 0.04 | 0.31 | 0.1 | 0.29 | 0.01 | 0.64 | 0.22 | 0.25 | 0.7 | 0.51 | 0.34 | 0.45 | 8.0 | 0.53 | 0.46 |
| Verify | 0.07 | 0.12 | 0.15 | 0.34 | 0 | 0.15 | -0.45 | 0.35 | 90:0- | 0.31 | 0.11 | 0.43 | -0.23 | 0.41 | 0.44 | 0.45 | 90:0 | 0.28 | 0.16 | -0.19 | 0.55 |
| PSI- BLAST | 1.80E-18 | 1.60E-05 | 5.40E-05 | 3.60E-17 | 5.40E-05 | 3.60E-05 | 90-E-06 | 3.60E-06 | 1.80E-15 | 0.00036 | 9.00E-07 | 1.80E-06 | 0.0045 | 0.00014 | 3.60E-20 | 9.00E-07 | 0.00018 | 1.10E-12 | 1.10E-21 | 0.00036 | 1.60E-05 |
| End | 4262 | 1127 | 1232 | 1439 | 1546 | 229 | 1691 | 1748 | 2061 | 2161 | 2562 | 2369 | 2458 | 7681 | 2788 | 3106 | 3191 | 3312 | 811 | 8 | 1021 |
| Start | 4134 | 1064 | 1169 | 1350 | 1455 | 155 | 6651 | 1991 | 1975 | 2079 | 2180 | 2304 | 2411 | 2592 | 2692 | 3039 | 3120 | 3225 | 716 | 852 | 932 |
| Chain | | | | | | | | | | | | | | | | | | | | | |
| 804 CI | 1klo | lncg | lncg | lncg | Incg | lncg | Incg | lncg | Incg | lncg | Incg | lncg |
| SEQ B B | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

| PDB annotation | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CELL |
|-----------------|---|---|---|---|---|---|---|---|--------------------------------|---|---|---|---|---|---|---|---|--------------------------------|---|---|----------------------------|
| Coumpound | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; CHAIN: A; |
| SeqFold | | | | | | | | | | | | | | | | | | | | | |
| PMF score | 97.0 | 6.0 | 90.0 | 91.0 | 0.64 | 9.4 | 0.27 | 20.0 | 0.3 | 9.0 | 0.49 | _ | 0 | 97.0 | 99.0 | 0.17 | 0.17 | 98.0 | 0.84 | 0.59 | - |
| Verify score | 90:0 | -0.16 | 0.53 | 0.21 | 0.26 | -0.17 | -0.5 | 0.24 | -0.4 | 0.39 | -0.03 | 0.56 | -0.01 | -0.24 | 0.52 | -0.2 | 0.31 | 0.01 | 0.26 | 0.4 | 0.39 |
| PSI- BLAST | 3.60E-06 | 1.80E-05 | 3.60E-16 | 5.40E-05 | 1.40E-06 | 5.40E-05 | 0.0045 | 1.80E-14 | 3.60E-06 | 5.40E-07 | 0.0079 | 1.80E-19 | 1.80E-06 | 0.0045 | 1.10E-06 | 0.0013 | 1.40E-10 | 5.40E-20 | 7.20E-05 | 7.20E-06 | 1.10E-35 |
| End AA | 1129 | 1234 | 1440 | 1547 | 1750 | 248 | 1960 | 2062 | 2264 | 2371 | 2458 | 2789 | 2898 | 3003 | 3105 | 3191 | 3313 | 812 | 216 | 7701 | 1234 |
| Start AA | 1065 | 8/11 | 1350 | 1481 | <i>L</i> 991 | 181 | 1912 | 5261 | 2180 | 2307 | 2412 | 7697 | 2832 | 2951 | 3041 | 3146 | 3225 | 911 | 853 | 932 | 1039 |
| Chain ID | В | В | м | м | В | В | В | В | В | м | В | В | В | В | В | В | В | В | В | В | Ą |
| 80g CI | Inci | Inci | Inci | 1nci | Inci | Inci | Inci | Inci | Inci | Inci | Inci | Inci | Inci | 1nci | lnci | Inci | 1nci | Inci | Inci | Inci | luci |
| SEQ B G | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

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|-----------------|------------------|---|---|---|---|---|---|--|---|---|---|---|--|---|--|---|---|---|---|---|---|
| PDB annotation | ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN |
| Coumpound | | N-CADHERIN: CHAIN: A; | N-CADHERIN: CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN: CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; |
| SeqFold | | | | | | | | | | | | | | | | | | | 120.25 | | |
| PMF | | - | 91.0 | 0.99 | 0.88 | - | 0.84 | 0.23 | | 6.0 | 0.45 | 68.0 | _ | - | 8.0 | 9.0 | 0.51 | _ | | _ | 66.0 |
| Verify score | | 0.53 | 0.1 | 0.28 | 0.02 | 0.46 | 0.2 | 80.0 | 0.31 | 0.25 | 0.02 | 0.23 | 0.25 | 0.32 | -0.03 | 90:0 | 0.28 | 0.23 | | 0.28 | 0.28 |
| PSI- BLAST | | 1.40E-31 | 1.80E-23 | 1.60E-58 | 3.60E-35 | 1.10E-33 | 7.20E-33 | 3.60E-22 | 9.00E-27 | 3.60E-31 | 1.60E-56 | 9.00E-31 | 3.60E-40 | 3.60E-35 | 9.00E-31 | 3.60E-40 | 1.30E-26 | 1.40E-31 | 3.60E-63 | 3.60E-63 | 9.00E-36 |
| End | | 1338 | 1440 | 1547 | 1652 | 1750 | 1861 | 354 | 1960 | 2062 | 2163 | 2264 | 2371 | 2473 | 2577 | 2683 | 450 | 2789 | 2897 | 2898 | 3003 |
| Start | | 1144 | 1251 | 1351 | 1455 | 1562 | 2991 | 173 | 1793 | 8681 | 1975 | 2079 | 2180 | 2300 | 2407 | 2488 | 256 | 2592 | 2691 | 2693 | 2825 |
| Chain ID | | ٧ | ٧ | V | ٧ | Y | ٧ | A | ٧ | ٧ | ٧ | ٧ | ٧ | Ą | A | ∢ | ∢ | ¥ | ٧ | ٧ | ٧ |
| PDB ID | | Incj | Incj | Incj | lncj | Incj | Incj | Incj | Incj | lncj. | Incj | lncj | lncj | lncj | lncj |
| SEQ B Si | | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

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| PDB annotation | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | SERINE PROTEASE FVIIA; BLOOD COAGULATION, SERINE | PROTEASE | SERINE PROTEASE FVIIA; BLOOD COAGULATION, SERINE | PROTEASE | | SERINE PROTEASE FVIIA; BLOOD COAGULATION, SERINE PROTEASE |
| Coumpound | N-CADHERIN; CHAIN: A; | COAGULATION FACTOR VIIA (LIGHT CHAIN); CHAIN: | L; COAGULATION FACTOR VIIA (HEAVY CHAIN); CHAIN: H; TRIPEPTIDYL INHIBITOR: CHAIN: C; | COAGULATION FACTOR VIIA (LIGHT CHAIN); CHAIN: | L; COAGULATION FACTOR VIIA (HEAVY CHAIN); | CHAIN: H; TRIPEPTIDYL INHIBITOR; CHAIN: C; | COAGULATION FACTOR VIIA (LIGHT CHAIN); CHAIN: L; COAGULATION FACTOR |
| SeqFold | | | | | | | | | | | | | | | | | | | |
| PMP score | _ | 8.0 | 0.82 | _ | _ | -0.03 | 0.21 | 0.36 | 96.0 | 0.01 | _ | 0.88 | _ | 0.57 | | -0.08 | | | -0.15 |
| Verify score | 0.35 | 0.16 | 0.35 | 99:0 | 9.0 | 0.35 | -0.28 | 80:0 | 0.36 | -0.13 | 0.39 | 0.35 | 0.48 | 89.0 | | 10.0 | | | 0.08 |
| PSI- BLAST | 9.00E-30 | 1.30E-30 | 1.30E-30 | 1.80E-39 | 1.80E-17 | 5.40E-10 | 1.10E-59 | 1.80E-35 | 7.20E-28 | 1.80E-25 | 1.10E-63 | 1.80E-34 | 3.60E-34 | 1.20E-21 | | 3.60E-13 | | | 7.20E-11 |
| End | 3105 | 3196 | 3313 | 3418 | 3523 | 3621 | 248 | 929 | 995 | 812 | 917 | 1022 | 1129 | 3947 | | 3976 | | | 4168 |
| Start AA | 2915 | 6202 | 3141 | 3228 | 3349 | 3473 | 39 | 390 | 467 | 573 | 717 | 827 | 932 | 3865 | | 3904 | | | 4082 |
| Chain ID | Ą | A | ٧ | A | ٧ | ٧ | Ą | ۷ | ٧ | ٧ | V | ٧ | A | ٦ | | 7 | | | ı. |
| PDB ID | Incj | 1ncj | Incj | 1ncj | Incj | lncj | Incj | lncj | Incj | Incj | lncj | Incj | Incj | 1gb 4gb | | lqfk | | | 1qfk |
| SEQ No. ID | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | | 808 | | | 808 |

| PDB annotation | | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BÎNDÎNG, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL |
|------------------|--|--|--|--|--|--|--|--|--|--|--|--|--|--|
| Coumpound | VIIA (HEAVY CHAIN); CHAIN: H; TRIPEPTIDYL INHIBITOR; CHAIN: C; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL: | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAJN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; |
| SeqFold score | | | | | | | | | | | | | | |
| PMF | | 0.13 | 0.27 | 0.45 | 0.4 | 0.62 | 0.25 | 69.0 | 0.11 | 0.07 | 0.31 | 60:0 | 89'0 | 99.0 |
| Verify score | | 0.33 | 0.24 | 0.04 | -0.03 | 0.54 | 0.3 | 0.45 | 0.14 | 0.35 | 0.41 | 0.2 | 0.07 | 90:0 |
| PSI- BLAST | | 7.20E-08 | 7.80E-20 | 1.30E-17 | 7.20E-08 | 1.30E-10 | 1.80E-21 | 1.30E-08 | 5.40E-07 | 2.60E-07 | 1.00E-12 | 1.40E-08 | 1.30E-12 | 3.60E-06 |
| End | | 1133 | 1133 | 1238 | 1238 | 1334 | 1444 | 1549 | | 226 | 1650 | 9591 | 1754 | 1754 |
| Start AA | | 1026 | 1041 | 1145 | 1711 | 1249 | 1350 | 1455 | 1455 | 155 | 1570 | 1589 | 1667 | 1690 |
| Chain | | | | | | | | | | | | | | |
| PDB ID | | 1suh | Isuh | lsuh | lsuh | 1suh | lsuh | 1suh | 1suh | Isuh | Isuh | lsuh | 1suh | Isuh |
| SEQ NO: | | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

| | _ | | | | · | | | , | | | | | | | _ |
|------------------|----------|--|--|--|--|--|--|--|--|--|--|--|--|---|---------------------------|
| PDB annotation | ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; |
| Coumpound | | EPITHELIAL CADHERIN; CHAIN: NULL; EPITHELIAL CADHERIN; |
| SeqFold score | | | | | | | | | | | | | | | |
| PMF score | | 0.48 | 0.39 | 0.13 | 0.18 | 1202.08 | 60:0 | 0.12 | 0.57 | 0.46 | 0.77 | 0.94 | 0.58 | 90:0 | 0.03 |
| Verify score | | -0.06 | -0.24 | -0.41 | 9.1 | 0.17 | 0.42 | 0.05 | -0.23 | -0.36 | 0.44 | 0.4 | 0.03 | -0.37 | -0.2 |
| PSI- BLAST | | 1.30E-14 | 3.60E-05 | 5.40E-07 | 1.60E-05 | 7.20E-18 | 2.60E-15 | 2167 3.60E-07 | 1.30E-14 | 3.60E-10 | 3.906-20 | 1.10E-08 | 3.90E-05 | 0.00011 | 3.60E-12 |
| End AA | | 1867 | 1868 | 252 | 1964 | 2066 | 2163 | 2167 | 2268 | 2268 | 2375 | 2375 | 2475 | 2477 | 2581 |
| Start AA | | EE1 | 1780 | 182 | 1898 | 1975 | 2084 | 2104 | 2178 | 2178 | 2280 | 2306 | 2395 | 2414 | 2488 |
| Chain D | | | | | | | | | | | | | | | |
| PDB ID | | Isuh | Isuh | Isuh | 1suh | 1suh | Isuh | lsuh | Isuh | Isuh | Isuh | 1suh | Isuh | Isuh | Isnh |
| SEQ O E E | | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

| PDB annotation | CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION ÜVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN: CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULN; CADHERN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION |
|-----------------|--|--|--|--|--|--|--|--|--|--|--|--|--|--|
| Coumpound | CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; |
| SeqFold | | | | | | | | | | | | | | |
| PMF | | 86.0 | 0.12 | 66.0 | 0.87 | 0.53 | 0.93 | 0.86 | 0.89 | 0.55 | 0.25 | 0.82 | 86:0 | 0.94 |
| Verify score | | 0.16 | 0.02 | 0.51 | 0.43 | -0.01 | 0.37 | -0.07 | 0.36 | 0.33 | 0.43 | 9.6 | 0.58 | 9.6 |
| PSI- BLAST | | 1.30E-13 | 2.60E-10 | 1.40E-23 | 2.60E-21 | 1.40E-08 | 1.20E-14 | 1.80E-05 | 2.60E-21 | 3.60E-06 | 3.90E-12 | 1.30E-13 | 3.90E-21 | 5.40E-05 |
| End | | 2581 | 2681 | 2793 | 2902 | 2902 | 3007 | 3007 | 3109 | 3109 | 3213 | 3317 | 3422 | 3422 |
| Start AA | | 2489 | 2591 | 2692 | 2806 | 2831 | 2914 | 2941 | 3026 | 3045 | 3120 | 3225 | 3330 | 3355 |
| Chain D | | | | | | | | | | | | | | |
| PDB CD | | lsuh | 1suh | 1suh | Isuh | Isuh | Isuh | 1suh | 1suh | Isuh | Isuh | Isuh | Isuh | lsuh |
| SEQ NO: | | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

| PDB annotation | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN: CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | PLASMINOGEN ACTIVATION | BLOOD COAGULATION FACTOR STUART FACTOR, BLOOD COAGULATION FACTOR, SERINE PROTEINASE, EPIDERMAL 2 GROWTH FACTOR LIKE DOMAIN | |
|------------------|--|--|--|--|--|--|--|--|--|--|--|--|--|
| Coumpound | EPITHELIAL CADHERIN; CHAIN: NULL; | T-PLASMINOGEN ACTIVATOR F1-G; 1TPG 7 CHAIN: NULL: 1TPG 8 | BLOOD COAGULATION FACTOR XA; CHAIN: L, C; | LECTIN (AGGLUTININ) WHEAT GERM AGGLUTININ (ISOLECTIN 2) 9WGA 3 |
| SeqFold score | | | | | | | | | | | | | |
| PMF | 0.65 | 0.24 | 0.3 | 0.19 | 0.57 | 0.95 | 0.72 | 0.47 | 0.57 | 0.18 | 0.59 | 0.1 | -0.2 |
| Verify score | 0.56 | 80.0 | -0.21 | -0.03 | 0.39 | -0.21 | 0.4 | 0.27 | 0.37 | 0.2 | 0.21 | -0.26 | 0.02 |
| PSI- BLAST | 6.50E-11 | 0.0001 | 9.00E-06 | 1.30E-15 | 3.90E-05 | 7.20E-25 | 1.00E-17 | 1.30E-07 | 5.20E-13 | 9.00E-07 | 1.30E-18 | 7.20E-11 | 4234 5.40E-12 |
| End | 3524 | 454 | 454 | 260 | 829 | 816 | 921 | 921 | 1026 | 1026 | 3940 | 3994 | 4234 |
| Start | 3435 | 363 | 401 | 467 | 230 | 716 | 826 | 854 | 930 | 656 | 3863 | 3904 | 4069 |
| Chain ID | | | | | | | | | | | | ے ا | A |
| PDB CD | 1suh | Isuh | 1suh | 1suh | Isuh | Isuh | lsth | 1suh | Isuh | Isuh | Itpg | 1xka | 9wga |
| SEQ No. | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 | 808 |

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|------------------|---|---|---|--|---|--|---|---|
| PDB annotation | | GROWTH FACTOR [ABU6, 20] MEGF4- GROWTH FACTOR, MURINE EPIDERMAL GROWTH FACTOR, DISULFIDE 2 CONNECTIVITIES, EGF- LIKE DOMAIN, REPEAT | COMPLEX (BLOOD COAGULATION/HEBITOR) ATTOPROLASE, SERANE PROTEINASE), PLASMA CALCUMB BINDING 2 GLYCOPROTEIN, COMPLEX (BLOOD COAGULATION/HEBITOR) | BLOOD COAGULATION BLOOD COAGULATION, EGF, HYDROLASE, SERINE PROTEASE | MEMBRANE PROTEIN LECTIN-LIKE, NEUROBIOLOGY, CELL-CELL ADHESION, CELL-CELL 2 RECOGNITION, ALTERNATIVE SPLICING, MEMBRANE PROTEIN | TRANSPORT PROTEIN SHBG; STERGOLI TRANSPORT, LAMININ G- LIKE DOMAIN, IELJYROCL, Z ANDROGEN BINDING PROTEIN (ABP), SEX STERGID BINDING PROTEIN 3 (SBP) | HYDROLASBAHYDROLASE INHIBITOR PROTEIN-PEPTIDE COMPLEX | HYDROLASEMYDROLASE INHIBITOR PROTEIN-PEPTIDE COMPLEX |
| Coumpound | | EPIDERMAL GROWTH FACTOR, CHAIN: NULL; | ACTIVATED PROTEIN C; CHAIN: C, L, D-PHE-PRO- MAI, CHAIN: P; | FACTOR VII; CHAIN: NULL; | NEUREXIN-I BETA; CHAIN: A, B, C, D, E, F, G, H; | SEX HORMONE-BINDING GLOBULIN; CHAIN: A; | DES-GLA FACTOR VIIA HEAVY CHAND; CHANN: H, I; DES-GLA FACTOR VIIA (LIGHT CHANN; CHANN: L, M; (DPN)-PHE-ARG; CHANN: C, D; PEPTIDE E-76; CHANN: X, Y; | DES-GLA FACTOR VIIA (ERAYY CHAN); CHANN; H I; DES-GLA FACTOR VIIA (LIGHT CHANN; CHANN; L M; (DPN)-PHE-ARC; CIANN; C, D; PEPTIDE E-76; CHANN; X, Y; |
| SeqFold score | | | | | | | | |
| PMF . | | 0.58 | -0.12 | 0.99 | 0.4 | 0.72 | 0.05 | -0.18 |
| Verify score | | 0.39 | 0.55 | 96.0 | 0.26 | 0.46 | 0.48 | 0.25 |
| PSI- BLAST | | 6.50E-12 | 6.50E-19 | 1.30E-11 | 1.305-26 | 2.60E-27 | 3.90E-21 | T.30E-13 |
| End | | 3984 | 4033 | 3987 | 3928 | 3934 | 4033 | 4344 |
| Start AA | | 3949 | 3943 | 3949 | 3771 | 3773 | 3944 | 4263 |
| Chain | | | n n | | ∢ . | ¥ | J | ᅱ |
| e e | | Ia3p | Jaut . | 16.69 | lo4r | 1d2s | Idva | ldva |
| SEQ NO: | | 608 | 68 | 608 | 608 | 808 | 808 | 808 |

| PDB annotation | SERINE PROTEINASE COAGULATION FACTOR II; FETOMODULIN, TA, CD14 AVITGENE, EGR-CARE, SERINE PROTEINASE, EGF-LIZE DOMAINS, ANTICOAGULANT COMPLEX, ANTICOAGULANT COMPLEX, ANTIFIBRINGLYTIC COMPLEX ANTIFIBRINGLYTIC COMPLEX | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADH2, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELAL. CADHERIN DOMAINS I AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN, | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADHS, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADHS, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADHS, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN, CALCIUM | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECAD12; CADHERIN, CELL |
|------------------|---|---|---|---|---|---|--|---|
| Coumpound | THROMBIN LIGHT CHAIN; CHAIN: A, B, C, D, THROMBIN HEAVY CHAIN; CHAIN: M, O, D; THROMBOMODULIN; CHAIN: I, K, L; THROMBIN HIMBITOR L-CLUJL-GUZ-L-ARM; CHAIN: E, F, G, H; | E-CADHERIN; CHAIN: Á, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; |
| SeqFold score | | | | | | | | |
| PMF score | -0.19 | - | 1202.08 | 6:0 | 0.82 | -1.41 | 96.0 | 0.99 |
| Verify | 0.06 | 0.26 | 0.22 | 0.45 | 0.27 | 0.1 | 0.21 | 0.19 |
| PSI- BLAST | 1.30E-11 | 3.60E-33 | 1.30E-32 | 3.60E-21 | 1.60E-49 | 1.30E-32 | 3.60E-33 | 1.60E-28 |
| End | 4336 | 1234 | 1338 | 1440 | 1547 | 1652 | 1750 | 1860 |
| Start AA | 4232 | 9901 | 1711 | 1279 | 1352 | 1460 | 1589 | 0691 |
| Chain | _ | ∢ | A | ¥ | ¥ | A | ¥ | ٧ |
| PDB CD | 1dx5 | 1edh | ledh | 1edh | ledh | ledh | 1edh | ledh |
| SEQ B B S | 608 | 608 | 809 | 608 | 808 | 809 | 608 | 608 |

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|------------------|---|---|---|---|---|---|---|---|---|
| PDB annotation | ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADHS, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM |
| Coumpound | | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B, |
| SeqFold score | | | | | - | | | | |
| PMF score | | 1 | 0 | 96:0 | 0.51 | 0.78 | _ | - | 0.86 |
| Verify score | | 0.32 | 0 | 0.26 | 0.3 | 0.24 | 0.18 | 0.32 | 0.07 |
| PSI- BLAST | | 3.60E-26 | 1.60E-20 | 3.60E-29 | 1.10E-50 | 1.30E-28 | 3.60E-48 | 1.60E-35 | 1.80E-29 |
| End | | 1960 | 354 | 2062 | 2163 | 2264 | 2371 | 2473 | 2577 |
| Start AA | | 1800 | 182 | 1898 | 1975 | 2104 | 2178 | 2306 | 2414 |
| Chain | | ¥ | < | ¥ | ∢ | v | ٧ | V | A |
| PDB CD | | 1edh | 1edh | 1edh | ledh | ledh | ledh | ledh | 1edh |
| SEQ NO: | | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 |

| | _ | | | | | | _ | | | | _ | | | | _ | | | | | | _ | _ | | _ | _ | | _ | | _ | _ | _ | |
|-----------------|-----------------|---|---|--------------------------|-------------------------------|---|--------------------------|-------------------------------|--------------------------|-----------------|--------------------------|-------------------------------|-------------------------------|---------------------------|-------------------------|-------------------------------|-------------------------------|---------------------------|-----------------|--------------------------|-------------------------------|-------------------------------|---------------------------|-------------------------|-------------------------------|-------------------------------|---------------------------|-----------------|--------------------------|-------------------------------|-------------------------------|--|
| PDB annotation | BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECAD12, CADHERIN, CELL | ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN | AND 2, ECAD12; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS 1 | ADHESION PROTEIN CALCIIM | BINDING PROTEIN | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS 1 | AND 2, ECAD12; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM | CELL A DIESTON BROTTEN | EPITHELIAL CADHERIN DOMAINS 1 | AND 2. ECAD12: CADHERIN. CELL | ADHESION PROTEIN, CALCIUM | BINDING PROTEIN | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS 1 | AND 2, ECAD12; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM | CELL ADDESION PROTEIN | EPITHELIA! CADHERIN DOMAINS 1 | AND 2, ECAD12; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM | BINDING PROTEIN | CELL ADHESION PROTEIN | EPITHELIAL CADHERIN DOMAINS 1 | AND 2, ECAD12; CADHERIN, CELL | ADHESION PROTEIN, CALCIUM BINDING PROTEIN |
| Coumpound | | E-CADHERIN; CHAIN: A, B; | | E-CADHERIN; CHAIN: A, B; | | | E-CADHERIN; CHAIN: A, B; | | | | E-CADHERIN; CHAIN: A, B; | | | | B-CADUEDIN: CHAIN: A D. | 'a 'u anno 'u anno a | | | | E-CADHERIN; CHAIN: A, B; | | | * | E-CADUEDIN: CHAIN: A D. | E-CADILLAM, CHAIN. A, B, | | | | E-CADHERIN; CHAIN: A, B; | | | |
| SeqFold | | | | | | | 120.62 | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.93 | | 96'0 | | | | | | | _ | | | | - | | | | | 0.94 | | | | 0.53 | 3 | | | | 0.64 | | | |
| Verify score | | 0 | | 0.1 | | | | | | | 0.47 | | | | 0.27 | į | | | | 0.31 | | | | 0.38 | 3 | | | | 91.0 | | | |
| PSI- BLAST | | 1.80E-38 | | 5.40E-32 | | | 1.80E-57 | | | | 1.80E-57 | | | | 7 20E-35 | | | | | 5.40E-29 | | | | 7 20E-25 | 7 | | | | 5.40E-28 | | | |
| End AA | | 2683 | | 2789 | | | 2895 | | | | 2898 | | | | 3003 | | | | | 3105 | | | | 450 | 3 | | | | 3197 | | | |
| Start AA | | 2488 | | 5619 | | | 2692 | | | | 2693 | | | | 2831 | i | | | | 2941 | | | | 206 | } | | | | 3046 | | | |
| Chain ID | | ¥ | - | A | | | Ą | | | | A | | | | Ą | | | | | ۷ | | | | A | | | | | Ą | | | |
| PDB ID | | ledh | | ledh | | | ledh | | | | ledh | | | - | ledh | | | | | led H | | _ | | ledh. | | | | | ledh | | | |
| SEQ NO: | | 608 | | 809 | | | 608 | | | | 608 | | | | 800 | ; | | | | <u></u> | | | | 800 | } | | | | 608 | | | |

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| PDB annotation | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIE, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIE, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIE, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADIE, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELAL CACHERIN DOMAINS I AND 2, ECADL2, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIE, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CACHERIN DOMAINS I AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CACHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN |
| Coumpound | E-CADHERIN; CHAIN: A, B; E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; |
| SeqFold | | | J | - | | | | | |
| PMF | -1.41 | 86:0 | _ | 0.3 | 0.83 | 0.82 | 0.27 | _ | _ |
| Verify score | 0.57 | 0.45 | 99.0 | 0.12 | 0.29 | 0.17 | -0.05 | 0.33 | 0.31 |
| PSI- BLAST | I.80E-32 | 1.80E-48 | 3.60E-30 | 1.80E-51 | 1.10E-29 | 3.60E-29 | 5.40E-22 | 1.10E-55 | 1.10E-32 |
| End AA | 3313 | 3418 | 3523 | 248 | 956 | 662 | 812 | 917 | 1022 |
| Start AA | 3120 | 3225 | 3355 | 39 | 406 | . 494 | 165 | 718 | 854 |
| Chain 10 | ¥ | ¥ | V | ⋖ | ¥ | ¥ | ∢ | ∢ | V |
| 8 E | ledh | 1cdh | ledh | 1edh | ledh | lodh | ledh | legh fl | legh |
| S a S | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 |

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|------------------|--|---|---|--|---------------------------|---------------------------|---------------------------|--|---|---|---|---|--------------------------------|---|--------------------------------|---|
| PDB annotation | EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADHS, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | MATRIX PROTEIN EXTRACELLULAR MATRIX, CALCIDIA-BINDING, GLYCOPROTEIN, 2 REPEAT, SIGNAL, MULTIGENE PAMILY, DISEASE MULTIGENE PAMILY, DISEASE MULTION, 3 EGF-LIKE DOMAIN, HUMAN PERILLIAN, PRAGMENT, MATRIX PROTEIN | CELL ADHESION PROTEIN EGF-LIKE DOMAIN, CELL ADHESION PROTEIN, TRANSMEMBRANE, 2 GLYCOPROTFIN | GLYCOPROTEIN GLYCOPROTEIN | GLYCOPROTEIN GLYCOPROTEIN | GLYCOPROTEIN GLYCOPROTEIN | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN | CELL ADHESTON PROTEIN CADHERIN INCG 13 |
| Coumpound | | E-CADHERIN; CHAIN: A, B; | FIBRILLIN; CHAIN: NULL; | P-SELECTIN; CHAIN: NULL; | LAMININ; CHAIN: NULL; | LAMININ; CHAIN: NULL; | LAMININ; CHAIN: NULL; | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 |
| SeqFold score | | | | | | | | | | | | | | | | |
| PMF | | 69:0 | 0.99 | 0.88 | 0.27 | -0.03 | -0.2 | 0.29 | 0.69 | 0.29 | 0.1 | 0.09 | 60.0 | 0.31 | 0.1 | 0.11 |
| Verify score | | 0.11 | 0.71 | 1.03 | -0.1 | 0.07 | 0.23 | 0.12 | 0.13 | 10.0 | 0.46 | 0.15 | -0.13 | 0.35 | 0.22 | 0.28 |
| PSI- BLAST | | 9.00E-32 | 1.80E-16 | 1.30E-11 | 1.10E-13 | 5.40E-21 | 3.60E-17 | 9.00E-06 | 0.00014 | 1.40E-14 | 0.00018 | 3.60E-05 | 9.00E-06 | 3.60E-06 | 3.60E-17 | 0.00036 |
| End | | 1129 | 4022 | 3988 | 4050 | 4075 | 4342 | 1127 | 1232 | 1439 | 1546 | 525 | 1650 | 1748 | 2061 | 2161 |
| Start AA | | . 656 | 3946 | 3949 | 3924 | 3954 | 4201 | 1062 | 1167 | 1350 | 1480 | 155 | 1299 | 1991 | 1970 | 2079 |
| Chain D | | ¥ | | | | | | | | | | | | | | |
| PDB CD | | 1edh | lem n | 1£sb | Ikio | 1kio | 1kjo | Incg | Incg | lncg | Incg | lncg | Jucg | lncg | Incg | Incg |
| Se Si | | 608 | 608 | 608 | 608 | 809 | 809 | 808 | 608 | 608 | 608 | 809 | 608 | 806 | 608 | 608 |

| PDB annotation | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN | CELL ADHESION PROTEIN CADHERIN | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN |
|------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|--|---|---|--------------------------------|--------------------------------|---|---|--------------------------------|
| Coumpound | N-CADHERIN; INCG 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | |
| PMF | 0.1 | 0.74 | 0.43 | 0.57 | 0.7 | 039 | 0.51 | 0.34 | 0.36 | 8.0 | 0.53 | 0.64 | 0.78 | 96.0 | 0.22 | 9.65 | 9.0 | 9.4 | 0.23 | 0.05 | 0.1 |
| Verify score | 80:0- | 0.41 | -0.27 | 0.34 | 0.44 | 0.35 | 0.45 | 90:0 | 0.33 | 91.0 | -0.19 | 0.38 | 90.0 | 90:0 | 0.43 | -0.08 | 0.35 | -0.17 | 80.0 | -0.25 | -0.11 |
| PSI- BLAST | 3.60E-12 | 1.80E-06 | 0.00036 | 1.60E-05 | 1.80E-19 | 0.00054 | 3.60E-06 | 1.80E-05 | 1.60E-11 | 7.20E-20 | 0.00018 | 5.40E-05 | 1.80E-06 | 5.40E-05 | 1.30E-13 | 0.00018 | 9.00E-07 | 1.60E-05 | 1.80E-16 | 0.0013 | 2264 1.30E-11 |
| End | 2263 | 2370 | 2458 | 2681 | 2788 | 2988 | 3106 | 3191 | 3311 | 811 | 06 | 1003 | 1129 | 1234 | 1440 | 1547 | 1750 | 248 | 2062 | 2163 | 2264 |
| Start AA | 2178 | 2304 | 2411 | 2593 | 2692 | 2913 | 3039 | 3120 | 3225 | 911 | 852 | 932 | 1065 | 1172 | 1350 | 1491 | 1991 | 181 | 1970 | 2116 | 2178 |
| Chain | | | | | | | | | | | | | В | В | m | æ | m | В | В | В | В |
| 908 CI | Incg | lncg | lncg | lncg | Incg | Incg | Inci | Inci | Inci | . Inci | Inci | Inci | Inci | Inci | Inci |
| SE OS | 608 | 808 | 808 | 608 | 809 | 608 | 608 | 608 | 608 | 608 | 608 | 808 | 608 | 809 | 608 | 808 | 608 | 808 | 809 | 608 | 809 |

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| PDB annotation | INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN |
| Coumpound | | N-CADHERIN; INCI 3 | N-CADHERIN; CHAIN: A; |
| SeqFold score | | | | | | | | | | | | | | | | | | , | | | |
| PMF score | | 0.75 | 0.58 | 90.0 | _ | 0.92 | 0.42 | 0.17 | 0.49 | 0.99 | 96:0 | 0.71 | 9.63 | _ | - | 0.54 | . 66'0 | _ | 0.21 | _ | 0.74 |
| Verify | | 0.17 | -0.I4 | 0 | 0.56 | 0.42 | 0.56 | -0.2 | 0.67 | 0.87 | 0.15 | -0.4 | 95.0 | 0.45 | 0.34 | 0.3 | 0.29 | 0.03 | 0.05 | 0.45 | -0.05 |
| PSI- BLAST | | 5.40E-07 | 60000 | 1.60E-05 | 3.60E-19 | 0.0036 | 5.40E-06 | 0.00036 | 1.80E-10 | 1.80E-08 | 1.80E-19 | 5.40E-05 | 1.80E-05 | 3.60E-36 | 5.40E-33 | 1.80E-22 | 3.60E-53 | 1.80E-34 | 5.40E-24 | 3.60E-33 | 3.60E-32 |
| End | | 12371 | 2458 | 2683 | 2789 | 3003 | 3105 | 3191 | 3313 | 3418 | 812 | 917 | 2201 | 1234 | 1338 | 1440 | 1547 | 1652 | 354 | 1750 | 1981 |
| Start AA | | 2307 | 2414 | 2620 | 2692 | 2942 | 3044 | 3146 | 3225 | 3354 | 715 | 862 | 932 | 6201 | 1147 | 1270 | 1351 | 1458 | 155 | 7951 | 1991 |
| Chain D | | В | В | æ | æ | В | В | В | м | В | 8 | В | В | V | A | A | ¥ | 4 | ٧ | ٧ | ٧ |
| PDB CD | | Inci | Inci | Inci | Inci | Inci | 1nci | Inci | Inci | Inci | Inci | Inci | 1nci | lncj | lncj | lncj | 1ncj | Incj | lncj | Incj | lncj |
| SEQ NO: | | 608 | 608 | 608 | 608 | 808 | 809 | 608 | 608 | 608 | 608 | 608 | 809 | 809 | 608 | 809 | 608 | 809 | 608 | 608 | 608 |

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| PDB annotation | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL |
| Coumpound | N-CADHERIN; CHAIN: A; | N-CADHERIN, CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; |
| SeqFold score | | | | | | | | | | | 120.25 | | | | | | | | | | |
| PMF score | 96'0 | 97.0 | 0.33 | 98.0 | _ | _ | 0.75 | 0.83 | 0.3 | 1 | | _ | 66.0 | - | 0.58 | 0.63 | 66.0 | - | 0.39 | 0.21 | 0.35 |
| Verify score | 0.31 | 0.42 | 0.11 | 0.48 | 0.17 | 0.27 | -0.1 | 0.14 | 0.25 | 0.29 | | 0.28 | 0.31 | 0.62 | -0.03 | 0.36 | 0.48 | 0.63 | 0.52 | -0.28 | 0.3 |
| PSI- BLAST | 7.20E-27 | 3.60E-28 | 7.20E-55 | 3.60E-30 | 5.40E-52 | 5.40E-36 | 7.20E-32 | 1.60E-41 | 3.60E-27 | 1.30E-32 | 5.40E-63 | 5.40E-63 | 3.60E-38 | 1.80E-29 | 1.40E-31 | 1.80E-34 | 7.20E-51 | 3.60E-32 | 3.60E-13 | 1.80E-57 | 1.80E-34 |
| End | 1960 | 2062 | 2163 | 2264 | 2371 | 2473 | 2577 | 2683 | 450 | 2789 | 2897 | 2898 | 3003 | 3105 | 3196 | 3313 | 3418 | 3523 | 3621 | 248 | 556 |
| Start AA | 1782 | 8681 | 0261 | 2079 | 2178 | 2300 | 2407 | 2488 | 256 | 2593 | 2691 | 2693 | 2825 | 2913 | 3039 | 3120 | 3225 | 3346 | 3433 | 39 | 390 |
| Chain | Ą | ٧ | ٧ | 4 | ٧ | V | ٧ | ٧ | ٧ | < | ∢ | ¥ | ¥ | ¥ | ¥ | ٧ | ¥ | Ą | ٧ | ٧ | Ą |
| PDB ID | lncj | Incj | Incj | Incj | Incj | 1ncj | Incj | Incj | 1ncj | Incj | lncj | Incj | Incj | lncj | Incj | 1ncj | Incj | lncj | lncj | Incj | lncj |
| SEQ No. | 608 | 608 | 608 | 608 | 608 | 808 | 808 | 608 | 608 | 608 | 608 | 608 | 809 | 608 | 608 | 608 | 808 | 608 | 608 | 809 | 608 |

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| PDB annotation | ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | COMPLEX (BLOOD) COACULATION/INHIBITOR) COACULATION/INHIBITOR) CHRISTMAS FACTOR; COMPLEX, INHIBITOR; HEMOGRILA/INFOR; BLOOD COACULATION 2 PLASMA, SERINE PROTEASE, CALCIUM BINDING, HYDROLASE, 3 GLYCOPROTEIN | SERNE PROTEASE FVIIA; FVIIA; BLOOD COAGULATION, SERINE PROTEASE | SERINE PROTEASE FVIIA; BLOOD COAGULATION, SERINE PROTEASE | SERNE PROTEASE FVIIA; BLOOD COAGULATION, SERINE PROTEASE | SERINE PROTEASE FVIIA; BLOOD COAGULATION, SERINE PROTEASE |
| Coumpound | | N-CADHERIN; CHAIN: A; | FACTOR IXA; CHAIN: C, L; D.PHE-PRO-ANG; CHAIN: I; | COAGULATION FACTOR VIIA (LIGHT CHAIN); CHAIN: L; COAGULATION FACTOR VIIA (HEAVY CHAIN); CHAIN: H; TRIPEPTIDYL INHBITOR, CHAIN: C | COAGULATION FACTOR VIIA (LIGHT CHAIN); CHAIN: L; COAGULATION FACTOR VIIA (HEAVY CHAIN); CHAIN: H; TREPETIDYL INHIBITOR; CHAIN: C | COAGULATION FACTOR VIIA (LIGHT CHAIN); CHAIN: L; COAGULATION FACTOR VIIA (HEAVY CHAIN); CHAIN: H; TRIPPTIDYL CHAIN: H; TRIPPTIDYL CHAIN: CHAIN: C | COAGULATION FACTOR VIIA (LIGHT CHAIN); CHAIN: L; COAGULATION FACTOR VIIA (HEAVY CHAIN); |
| SeqFold | | | | | | | | | | | |
| PMF score | | 66.0 | 0.18 | 1 | 0.88 | 1 | -0.19 | -0.19 | 0.57 | -0.17 | -0.17 |
| Verify score | | 0.37 | 0.02 | 0.23 | 0.34 | 0.39 | 0.01 | 0.2 | 99.0 | 0 | 0.37 |
| PSI- BLAST | | 9.00E-30 | 1.80E-25 | 7.20E-62 | 1.80E-34 | 1.10E-34 | 1.40E-10 | 1.30E-11 | 1.20E-21 | 5.40B-14 | 7.20E-13 |
| End | | 799 | 812 | 917 | 1022 | 1129 | 4312 | 4001 | 4033 | 4202 | 4344 |
| Start | | 467 | 57.1 | 717 | 827 | 932 | 4224 | 3943 | 3951 | 4121 | 4267 |
| Chain | | V | Ą | Ą | Ą | Ą | , | 1 | L) | 1 | T. |
| 80g En | ľ | Incj | Incj | Incj | Incj | Incj | Τρξ | 1qfk | lqfk | 1qfk | 1qfk |
| SEQ EQ EQ | | 608 | 608 | 608 | 608 | 608 | 808 | 608 | 608 | 608 | 608 |

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|-----------------|--|---|--|--|--|--|--|--|--|--|--|--|--|--|
| PDB annotation | | COAGULATION FACTOR SERINE PROTEINASE, BLOOD COAGULATION, COAGULATION FACTOR | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL |
| Coumpound | CHAIN: H; TRIPEPTIDYL NHIBITOR; CHAIN: C; | COAGULATION FACTOR IX; CHAIN: A; COAGULATION FACTOR IX; CHAIN: B; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPTHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL: |
| SeqFold | | | | | | | | | | | | | | |
| PMF | | -0.19 | 0.27 | 0.93 | 0.45 | 0.62 | 0.13 | 0.04 | 0.63 | 0.07 | 0.31 | 0.13 | 99.0 | 0.75 |
| Verify score | | 0.03 | 0.24 | -0.06 | 0.04 | 0.54 | 0.28 | 0.37 | 0.45 | 0.35 | 0.41 | -0.2 | 0.07 | 0.17 |
| PSI- BLAST | | 7.80E-14 | 7.80E-20 | 1.60E-07 | 1.30E-17 | 1.30E-10 | 0.0013 | 1.80E-19 | 1.30E-08 | 2.60E-07 | 1.00E-12 | 9.00E-09 | 1.30E-12 | 1754 3.60E-06 |
| End AA | | 4001 | 1133 | 1133 | 1238 | 1334 | 1342 | 1444 | 1549 | 922 | 1650 | 9591 | 1754 | 1754 |
| Start AA | | 3951 | 1041 | 1066 | 1145 | 1249 | 1279 | 1350 | 1455 | 155 | 1570 | 1589 | 1991 | 1690 |
| Chain D | | В | | | | | | | | | | | | |
| PDB CD | | 即 | Isuh | 1suh | Isuh | Isuh | Isuh | lsuh | Isuh | Isuh | 1suh | Isuh | 1suh | ųns į |
| SEQ NO: | | 608 | 608 | 608 | 608 | 608 | 809 | 608 | 608 | 608 | 608 | 808 | 809 | 608 |

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|------------------|----------|--|--|--|--|--|--|--|--|--|--|--|--|--|---------------------------|
| PDB annotation | ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN: CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORUTIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; |
| Coumpound | | EPITHELIAL CADHERIN; CHAIN: NULL; | BPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; |
| SeqFold score | | | | | | | | | | | | | | | |
| PMF score | | 0.48 | 0.45 | 0.13 | 60:0 | 0.4 | 0.77 | 0.94 | 0.58 | 0.25 | 0.15 | 86:0 | 0.12 | 0.99 | 0.87 |
| Verify score | | -0.06 | -0.18 | -0.41 | 0.42 | -0.37 | 0.44 | 0.35 | 0.03 | -0.04 | -0.37 | 0.16 | 0.02 | 0.42 | 0.43 |
| PSI- BLAST | | 1.30E-14 | 3.60E-05 | 1.80E-06 | 2.60E-15 | 1.30E-15 | 3.90E-20 | 2375 3.60E-09 | 3.90E-05 | 2477 3.60E-05 | 1.80E-12 | 1.30E-13 | 2.60E-10 | 3.60E-23 | 2902 2.60E-21 |
| End AA | | 1867 | 1868 | 252 | 2163 | 2268 | 2375 | 2375 | 2475 | 2477 | 2581 | 2581 | 2681 | 2793 | 2902 |
| Start AA | | 1771 | 1800 | 182 | 2084 | 2178 | 2280 | 2306 | 2395 | 2414 | 2488 | 2489 | 2591 | 2692 | 2806 |
| Chain D | | 0 | | | | | | | | | | | | | |
| PDB CD | | Isuh | Isuh | Isuh | 1suh | 1suh | 1suh | lsuh | 1suh | Isuh | 1suh | 1suh | Isuh | lsuh | Isuh |
| S e ŝ | | 608 | 608 | 808 | 608 | 608 | 608 | 608 | 608 | .608 | 608 | 66 | 608 | 608 | 808 |

| PDB annotation | CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN: CADHERIN, CALCIUM BINDING, CELL ADHESION |
|------------------|--|--|--|--|--|--|--|--|--|--|--|--|--|--|
| Coumpound | CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; |
| SeqFold score | | | | | | | | | | | | | | |
| PMF score | | 0.25 | 0.93 | 98'0 | 0.89 | 0.72 | 0.28 | 0.25 | 0.82 | 86.0 | 0.93 | 0.65 | 0.24 | 0.19 |
| Verify score | | 0.01 | 0.37 | -0.07 | 0.36 | 0.4 | 0.1 | 0.43 | 0.6 | 0.58 | 99.0 | 0.56 | 0.08 | -0.6 |
| PSI- BLAST | | 3.60E-09 | 1.20E-14 | 1.80E-06 | 2.60E-21 | 3.60E-06 | 0.0013 | 3.90E-12 | 1.10E-14 | 3.90E-21 | 1.30E-09 | 6.50E-11 | 0.0001 | 1.60E-05 |
| End AA | | 2902 | 3007 | 3007 | 3109 | 3109 | 3185 | 3213 | 3317 | 3422 | 3422 | 3524 | 454 | 454 |
| Start AA | | 2831 | 2914 | 2941 | 3026 | 3046 | 3120 | 3120 | 3225 | 3330 | 3355 | 3435 | 363 | 406 |
| Chain ID | | | | | | | | | | | | | | |
| PDB ID | | 1suh | 1suh | Isuh | Isuh | lsuh | 1suh | 1suh | Isuh | 1suh | 1suh | 1suh | 1suh | Isuh |
| SEQ NO: | | 608 | 608 | 608 | 608 | 608 | 608 | 809 | 809 | 809 | 803 | 608 | 608 | 608 |

| PDB annotation | CELL ADHESION UVOMORULN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | PLASMINOGEN ACTIVATION | BLOOD COAGULATION FACTOR STUART FACTOR, BLOOD COAGULATION FACTOR, SERINE PROTEINASE, EPIDERMAL 2 GROWTH FACTOR LIKE DOMAIN | | COMPLEX (BLOOD COAGULATION/HIBHTOR) AUTOPROTHROMBIN ID; PLASMA, CALCIUM BINDING; 2 GLYCOPROTEN, COMPLEX (BLOOD COAGULATION/HIBHTOR) | BLOOD COAGULATION, SERINE PROTEASE, COMPLEX, CO-FACTOR, 2 RECEPTOR BNZYME, INHIBITOR, GLA, EGF, 3 COMPLEX (SERINE PROTEASECOPACTORILIGAND) |
|------------------|---|--|--|--|--|--|--|--|--|---|--|
| Coumpound | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | T-PLASMINOGEN ACTIVATOR F1-G; 1TPG 7 CHAIN: NULL; 1TPG 8 | BLOOD COAGULATION FACTOR XA; CHAIN: L, C; | LECTIN (AGGLUTININ) WHEAT GERM AGGLUTININ (ISOLECTIN 2) 9WGA 3 | ACTIVATED PROTEIN C; CHAIN: C, L, D-PHE-PRO- MAI; CHAIN: P; | BLOOD COAGULATION FACTOR VILA; CHAIN: I., H; SOLUBLE TISSUE FACTOR; CHAIN: T, U; D-PHE-PHE- ARG- |
| SeqFold score | | | | | | | | | | | |
| PMF | 0.19 | 0.57 | 0.95 | 0.72 | 0.45 | 0.57 | 0.59 | -0.19 | -0.2 | -0.12 | 0.07 |
| Verify score | -0.03 | 0.39 | -0.21 | 0.4 | 0.17 | 0.37 | 0.21 | 0.15 | 0.05 | 0.55 | 60.0 |
| PSI- BLAST | 1.30E-15 | 3.90E-05 | 1.40E-23 | 1.00E-17 | 5.40E-07 | 5.20E-13 | 1.30E-18 | 5.40E-12 | 3.60E-10 | 6.50E-19 | 1.40E-12 |
| End | 260 | 859 | 918 | 921 | 126 | 1026 | 4026 | 4348 | 4337 | 3947 | 3897 |
| Start | 467 | 290 | 912 | 826 | 854 | 930 | 3949 | 4267 | 4166 | 3857 | 3831 |
| Chain | | | | | | | | ı | A | 1 | ب |
| ag ar | Isuh | 1suh | lsuh | 1suh | lsuh | lsuh | 1tpg | lxka | 9wga | laut | ldan |
| SEQ B B SE | 608 | 608 | 608 | 608 | 808 | 808 | 809 | | 608 | 808 | 608 |

| PDB annotation | | BLOOD COAGULATION, SERINE PROTEASE, COMPLEX, CO-FACTOR, 2 RECEPTOR ENZYME, INHIBITOR, GLA, EGF, 3 COMPLEX (SERINE | PROTEASE/COFACTOR/LIGAND) | HYDROLASE/HYDROLASE INHIBITOR PROTEIN-PEPTIDE COMPLEX | | HYDROLASE/HYDROLASE INHIBITOR | PROTEIN-PEPTIDE COMPLEX | | | HYDROLASE/HYDROLASE INHIBITOR PROTEIN-PEPTIDE COMPLEX | | | HYDROLASE/HYDROLASE INHIBITOR | PROTEIN-PEPTIDE COMPLEX | | | | HYDROLASE/HYDROLASE INHIBITOR | |
|-----------------|---|---|--|---|--|-------------------------------|---|--|----------------------------------|---|--|--|-------------------------------|--------------------------|--------------------------|----------------------------|-------|-------------------------------|--|
| Coumpound | CHLOROMETHYLKETONE (DFFRCMK) WITH CHAIN: C; | BLOOD COAGULATION FACTOR VIIA; CHAIN: L, H; SOLUBLE TISSUE FACTOR; CHAIN: T, U; D-PHE-PHE- | ARG- CHLOROMETHYLKETONE (DFFRCMK) WITH CHAIN: C; | DES-GLA FACTOR VIIA (HEAVY CHAIN); CHAIN: H, I; DES-GLA FACTOR VIIA | (LIGHT CHAIN); CHAIN: L, M; (DPN)-PHE-ARG; CHAIN: C, D; PEPTIDE E-76; CHAIN: v, v. | DES-GLA FACTOR VIIA | (HEAVY CHAIN); CHAIN: H, I; DES-GLA FACTOR VIIA | (LIGHT CHAIN); CHAIN: L, M: (DPN)-PHE-ARG: CHAIN: | C, D; PEPTIDE E-76; CHAIN: X, Y; | DES-GLA FACTOR VIIA (HEAVY CHAIN); CHAIN: H, | I; DES-GLA FACTOR VIIA (LIGHT CHAIN); CHAIN: L, | M; (DPN)-PHE-ARG; CHAIN: C, D; PEPTIDE E-76; CHAIN: | DES-GLA FACTOR VIIA | (HEAVY CHAIN); CHAIN: H, | (LIGHT CHAIN); CHAIN: L, | C. D. PEPTIDE E-76: CHAIN: | X, Y; | DES-GLA FACTOR VIIA | I; DES-GLA FACTOR VIIA (LIGHT CHAIN); CHAIN: L, |
| SeqFold | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.07 | | 0.15 | | 0.05 | | | | -0.07 | | | -0.15 | | | | | -0.19 | |
| Verify score | | 0.1 | | -0.08 | | 0.48 | | | | 0.12 | | | 0.05 | | | | | 0.25 | |
| PSI- BLAST | | 3.60E-14 | | 1.40E-12 | | 3.90E-21 | | | | 3.60E-14 | | | 3.60E-12 | | | | | 1.30E-13 | |
| Fud AA | | 39.76 | | 3897 | | 3947 | | | | 3976 | | | 4168 | | | | | 4259 | |
| Start | | 3900 | | 3831 | | 3858 | | | | 3900 | | | 4078 | | | | | 4170 | |
| Chain ID | | Г | | ı | | l, | | | | ı | | | r | | | | | Т | |
| 808 a | | 1dan | | ldva | | Idva | | | | ldva | | | Idva | | | | | Bybl | |
| S e S | | 608 | | 608 | | 808 | | | | 808 | | | S08 | | | | | 608 | |

| PDB annotation | | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIE; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADHS, CADHERIN, CELL ADHESION PROTEIN, CALCIUM RINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADIE; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADD2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN, | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADDS; CADHERIN, CELL ADHESION PROTEIN, CALCIUM RINNING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIE; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN, | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL |
|-----------------|---|---|---|---|---|--|---|--|---|
| Coumpound | M; (DPN)-PHE-ARG; CHAIN: C, D; PEPTIDE E-76; CHAIN: X, Y; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN, CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; |
| SeqFold | | | | | | | | | |
| PMF | | _ | 96:0 | 0.93 | 0.89 | 0.65 | -1.41 | 0.25 | 66.0 |
| Verify score | | 0.35 | 0.16 | 0.23 | 0.3 | 0.03 | 0.19 | -0.18 | 0.21 |
| PSI- BLAST | | 1.106-33 | 1338 9.00E-30 | 1.60E-20 | 3.60E-54 | 7.20B-32 | 3.60E-33 | 3.60E-28 | 1960 1.80E-27 |
| End | | 1234 | 1338 | 1440 | 1547 | 1652 | 1750 | 1860 | 1960 |
| Start | | 1026 | 1171 | 1279 | 1352 | 1455 | 1589 | 1690 | 1780 |
| Chain | | ⋖ | ∢ | ∢ | ∢ . | ¥ | ¥ | ∢ | ٧ |
| 802 E1 | | ledh | 1edh | 1edh | 1edh | ledh | 1cdh | ledh | ledh |
| SEQ B B S | | 808 | 808 | 608 | 608 | 608 | . 608 | 608 | 608 |

| PDB annotation | ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2, CADHERIN, CELL ADHESION RROTEIN, CALCIUM BINDING RROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIE, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN, CALCIUM | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIE, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD 12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM |
|-----------------|--|---|---|---|---|--|---|--|---|
| Coumpound | | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; |
| SeqFold | | | | | | | | | |
| PMF | | 0.07 | 0.94 | 0.34 | 0.92 | _ | -1.41 | 98.0 | 0.75 |
| Verify score | | 0.17 | 0.3 | 0.13 | 0.19 | 0.08 | 0.37 | 0.07 | 0.14 |
| PSI- BLAST | | 5.40E-20 | 1.80E-30 | 1.80E-50 | 9.00E-29 | 1.80E-38 | 1.80E-32 | 3.60E-29 | 1.60E-39 |
| End AA | | 354 | 2062 | 2163 | 2264 | 2371 | 2473 | 72577 | 2683 |
| Start | | 182 | 8681 | 1975 | 2104 | 2178 | 2306 | 2414 | 2488 |
| Chain ED | | ∢ | ∀ | < | × | < | ¥ | ∢ | 4 |
| PDB CI | | 1edh | 1ed | ledh | 1edh | ledh | ledh | ledh | ledh |
| SEQ NO ES | | 608 | 608 | 809 | 608 | 608 | 608 | 608 | 608 |

| PDB annotation | BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM | BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCTUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 | AND 2, ECADIZ; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADHESIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12, CADHERIN, CELL AND ADHESION PROTEIN, CALCIUM BARDANG PROTEIN, CALCIUM | CELL ADHESION PROTEIN EPITHELLAL CADHERIN DOMAINS I AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCTUM BINDING PROTEIN, | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS 1 AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN |
|------------------|-----------------|---|-----------------|---|---|--|---|--|--|--|---|
| Coumpound | | E-CADHERIN; CHAIN: A, B; | | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; |
| SeqFold score | | | | 120.62 | | | | | | | |
| PMF score | | 66.0 | | | _ | 1202.08 | | 0.94 | 0.41 | 9.0 | 0.59 |
| Verify score | | 0.33 | | | 0.52 | 0.46 | | 0.31 | 0.15 | 0.28 | 0.15 |
| PSI- BLAST | | 7.20E-31 | | 5.40E-58 | 5.40E-58 | 1.80E-33 | | 1.80E-28 | 5.40E-24 | 1.80E-27 | 1.80E-28 |
| End | | 2789 | | 2895 | 2898 | 3003 | | 3105 | 450 | 3191 | 3313 |
| Start | | 2619 | | 2692 | 2693 | 2831 | | 2941 | 296 | 3045 | 3147 |
| Chain ID | | ¥ | | ∢ | v | ٧ | | Ą | A | A | V |
| 80 a | | ledh | | He dh | ledh | ledh | | ledh | ledh | ledh | ledh |
| SEQ No. | | 608 | | 608 | 809 | 808 | | 608 | 608 | 608 | 809 |

| PDB annotation | CELL ADHESION PROTEIN EPITHELAL. CADHERIN DOMAINS I AND 2, ECADI-2, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL. CADHERIN DOMAINS I AND 2, ECAD 12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPTHELIAL CADHERIN DOMAINS I AND 2, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIE, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2. ECAD 12. CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD12; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADI2; CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | MATRIX PROTEIN EXTRACELLULAR |
|------------------|--|---|--|---|---|--|---|---|------------------------------|
| Coumpound | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN; A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | FIBRILLIN; CHAIN: NULL; |
| SeqFold score | | | | | | | | | |
| PMF | 86:0 | _ | 0.3 | 0.89 | 0.77 | _ | _ | 0.52 | 0.48 |
| Verify | 0.53 | 0.47 | 0.12 | 0.31 | 0.5 | 0.33 | 0.14 | 0.24 | 90.0 |
| PSI- BLAST | 1.40E-35 | 1.80E-16 | 3.60E-53 | 5.40E-30 | 3.60E-27 | 1.10E-57 | 1.80E-33 | 1.80E-30 | 3.60E-16 |
| End | 3418 | 3523 | 248 | 556 | 662 | 716 | 1022 | 1129 | 3931 |
| Start | 3225 | 3355 | 39 | 401 | 465 | 718 | 854 | 626 | 3860 |
| Chain El | ∢ | ď | ¥ | ∢. | ¥ | V | ¥ | V | |
| 804 E | ag di | . 1egh | legh | ledh . | ledi | ledi del | ledh | 1edh | <u>E</u> |
| S e S | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 809 |

| PDB annotation | MATRIX, CALCIUM-BINDING, GLYCOPROTER), 2 REBEAT, SIGNAL, MULTIGENE FAMILY, DISEASE MUTATION, 3 EGF-LIKE DOMAIN, HUMAN FIRILLIN-I FRAGMENT, MATRIX PROTEIN | MATRIX PROTEIN EXTRACELLULAR MATRIX, CALCUMABINDING, GLYCOPROTEIN, 2 REPEAT, SIGNAL, MULTGENE FAMILY, DISEAE, MUTATION, 3 EGF-LIKE DOMAIN, HUMAN FIBRILLIN-I FRAGMENT, | BLOOD CLOTTING COMPLEX(SERNE PROTEASEOCA-CIOSLICAND), BLOOD COAGULATION, 2 SERNE PROTEASE, COMPLEX, CO-FACTOR, GLA, EGF, COMPLEX, CO-FACTOR, GLA, EGF, COMPLEX (SERNE 4 PROTEASE/CORFATOR/LICAND), BLOOD CLOTTING | BLOOD CLOTTING COMPLEX(SERNE) RROTEASED/CAPACIOR/LGAND), BLOOD COAGULATION, 2 SERNE PROTEASE, COMPLEX, CO-FACTOR, GLA, EGG, COMPLEX, CORPETOR, GLA, EGG, COMPLEX (SERNE 4 PROTEASE/CORPACIOR/LIGAND), HALODO CLOTTING | GLYCOPROTEIN GLYCOPROTEIN | GLYCOPROTEIN GLYCOPROTEIN | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 |
|------------------|---|---|--|---|---------------------------|---------------------------|---|---|--|---|--|
| Coumpound | | FIBRILLN; CHAIN: NULL; | BLOOD COAGULATION FACTOR VIIA; CHAIN: L; BLOOD COAGULATION FACTOR VIIA; CHAIN: H; SOLUBLE TISSUE FACTOR; CHAIN: T; \$1.15; CHAIN: I; | BLOOD COAGULATION FACTOR VIIA; CHAIN: L; BLOOD COAGULATION FACTOR VIIA; CHAIN: H; SOLUBLE TISSUE FACTOR; CHAIN: T; 51.15; CHAIN: I; | LAMININ; CHAIN: NULL; | LAMININ; CHAIN: NULL; | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 |
| SeqFold score | | | | | | | | | | | |
| PMF | | -0.18 | -0.01 | -0.19 | -0.2 | -0.2 | 0.63 | 0.87 | 0.3 | 0.72 | 60:0 |
| Verify | | 0.02 | 0.12 | 0.2 | 0.07 | 0.07 | 0.12 | 0.15 | 0.34 | | 0.15 |
| PSI- BLAST | | 9.00E-14 | 3.60E-14 | 1.30E-13 | 1.80E-17 | 1.80E-18 | 1.60E-05 | 5.40E-05 | 3.60E-17 | S.40E-05 | 3.60E-05 |
| End AA | | 4217 | 3976 | 4259 | 4228 | 4262 | 1127 | 1232 | 1439 | 1546 | 229 |
| Start | | 4126 | 3900 | 4170 | 4074 | 4134 | 1064 | 1169 | 1350 | 1455 | 155 |
| Chain D | | | -1 | ı | | | | | | | |
| EDB CD | u | lem n | ·1fak | 1fak | . 1klo | 1klo | lncg | Boul | Boul | Jucg | lncg |
| SEQ NO: | | 808 | 608 | 608 | 808 | ŝ | 608 | 608 | 608 | 809 | 608 |

| PDB annotation | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN |
|----------------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|--------------------------------|
| Coumpound | N-CADHERIN; INCG 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 |
| SeqFold | | | | | | | | | | | | | | | | | | | | | |
| PMF | 0.04 | 0.31 | 0.1 | 0.29 | 0.01 | 0.64 | 0.22 | 0.25 | 0.7 | 0.51 | 0.34 | 0.45 | 8.0 | 0.53 | 0.46 | 0.78 | 6.0 | 90.0 | 0.16 | 9.64 | 0.4 |
| Verify | -0.45 | 0.35 | -0.06 | 0.31 | 0.11 | 0.43 | -0.23 | 0.41 | 0.44 | 0.45 | 90:0 | 0.28 | 0.16 | -0.19 | 0.55 | 90:0 | -0.16 | 0.53 | 0.21 | 0.26 | -0.17 |
| PSI- BLAST | 9.00E-06 | 3.60E-06 | 1.80E-15 | 0.00036 | 9.00E-07 | 1.80E-06 | 0.0045 | 0.00014 | 3.60E-20 | 9.00E-07 | 0.00018 | 1.10E-12 | 1.10E-21 | 0.00036 | 1.60E-05 | 3.60E-06 | 1.80E-05 | 3.60E-16 | 5.40E-05 | | 5.40E-05 |
| End | 1651 | 1748 | 2061 | 2161 | 2362 | 2369 | 2458 | 2681 | 2788 | 3106 | 3191 | 3312 | 118 | 06 | 1021 | 1129 | 1234 | 1440 | 1547 | | 248 |
| Start AA | 1599 | 1991 | 1975 | 2079 | 2180 | 2304 | 2411 | 2592 | 7692 | 3039 | 3120 | 3225 | 716 | 852 | 932 | 1065 | 1178 | 1350 | 1481 | 1667 | 181 |
| Chain | | | | | | | | | | | | | | | | æ | m | æ | ш | ш | В |
| PDB ID | Incg | Incg | Incg | lncg | Incg | lncg | lncg | Incg | lncg | lncg | lncg | lncg | Incg | lncg | lncg | Inci | Inci | Inci | Inci | Inci | 1nci |
| SEQ Sign | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 808 | 608 | 608 | 608 | 809 | 608 | 608 | 808 | 608 | 608 | 808 | 608 | 808 |

| PDB annotation | INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN | CELL ADHESION PROTEIN CADHERIN | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN |
|------------------|---------|---|---|---|---|---|---|---|---|--------------------------------|--------------------------------|---|---|---|---|---|---|---|---|---|---|
| Coumpound | | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; 1NCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; 1NCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; CHAIN: A; |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.27 | 0.07 | 0.3 | 9.0 | 0.49 | - | 0 | 0.78 | 99.0 | 0.17 | 0.17 | 0.88 | 0.84 | 0.59 | 1 | - | 0.16 | . 66.0 | 0.88 | 1 |
| Verify | | -0.5 | 0.24 | 4.0 | 0.39 | -0.03 | 0.56 | -0.01 | -0.24 | 0.52 | -0.2 | 0.31 | 10:01 | 0.26 | 0.4 | 0.39 | 0.53 | 1.0 | 0.28 | 0.02 | 0.46 |
| PSI- BLAST | | 0.0045 | 1.80E-14 | 3.60E-06 | 5.40E-07 | 6,000 | 1.80E-19 | 1.80E-06 | 0.0045 | 1.10E-06 | 0.0013 | 1.40E-10 | 5.40E-20 | 7.20E-05 | 7.20E-06 | 1.10E-35 | 1.40E-31 | 1.80E-23 | 1.60E-58 | 3.60E-35 | 1.10E-33 |
| End | | 0961 | 2062 | 2264 | 2371 | 2458 | 2789 | 2898 | 3003 | 3105 | 3191 | 3313 | 812 | 917 | 1022 | 1234 | 1338 | 1440 | 1547 | 1652 | 1750 |
| Start | | 1912 | 1975 | 2180 | 2307 | 2412 | 2692 | 2832 | 2951 | 3041 | 3146 | 3225 | 716 | 853 | 932 | 1039 | 1144 | 1251 | 1351 | 1455 | 1562 |
| Chain | | В | В | B | В | В | В | В | В | В | В | В | В | В | В | ¥ | ¥ | V | Ą | Ą | ٧ |
| EDB CD | | Inci | Inci | Inci | luci | Inci | Inci | 1nci | Inci | Inci | Inci | Inci | lnci | lnci | Inci | lncj | Incj | Incj | Incj | 1ncj | Incj |
| SEQ NO E | | 608 | 608 | 608 | 608 | 608 | 809 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 808 |

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|------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|----------------------------|
| PDB annotation | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL |
| Coumpound | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; |
| SeqFold score | | | | | | | | | | | | | 120.25 | | | | | | | | |
| PMF | 0.84 | 0.23 | _ | 6.0 | 0.45 | 68.0 | _ | _ | 9.0 | 9.0 | 0.51 | _ | | _ | 66'0 | I | 8.0 | 0.82 | _ | - | -0.03 |
| Verify | 0.2 | 80:0 | 16.0 | 0.25 | 0.02 | 0.23 | 0.25 | 0.32 | -0.03 | 90:0 | 0.28 | 0.23 | | 0.28 | 0.28 | 0.35 | 91.0 | 0.35 | 99.0 | 9'0 | 0.35 |
| PSI- BLAST | 7.20E-33 | 3.60E-22 | 9.00E-27 | 3.60E-31 | 1.60E-56 | 9.00E-31 | 3.60E-40 | 3.60E-35 | 9.00E-31 | 3.60E-40 | 1.30E-26 | 1.40E-31 | 3.60E-63 | 3.60E-63 | 9.00E-36 | 9.00E-30 | 1.30E-30 | 1.30E-30 | 1.80E-39 | 1.80E-17 | 5.40E-10 |
| End AA | 1861 | 354 | 0961 | 2062 | 2163 | 2264 | 2371 | 2473 | 2577 | 2683 | 450 | 2789 | 2897 | 2898 | 3003 | 3105 | 3196 | 3313 | 3418 | 3523 | 3621 |
| Start AA | 1991 | 173 | 1793 | 1898 | 1975 | 2079 | 2180 | 2300 | 2407 | 2488 | 256 | 2592 | 2691 | 2693 | 2825 | 2915 | 3039 | 3141 | 3225 | 3349 | 3473 |
| Chain D. | A | ¥ | A | V | A | A | Ą | A | A | A | ¥ | ¥ | ¥ | A | ¥ | ¥ | ¥ | ٧ | ٧ | ۷ | V |
| PDB ID | Incj | Incj | Incj | Incj | Incj | Incj | 1ncj | Incj | Incj | Incj | Incj | lncj | Incj | Incj | lncj | Incj | Incj | Incj | Incj | lncj | Inci |
| SEQ NO: | 809 | 808 | 608 | 808 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 808 | 808 | 608 | 608 | 608 | 808 | 608 |

| PDB annotation | ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | SERINE PROTEASE FVIIA; FVIIA; | BLOOD COAGULATION, SERINE | PROTEASE | | | SERINE PROTEASE FVIIA; FVIIA; | PROTEASE | | | SERINE PROTEASE FVIIA; FVIIA; | BLOOD COAGULATION, SERINE | LINGIFUSE | | | CELL ADHESION UVOMORULIN; | CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; | CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL |
|----------------|------------------|---|---|---|---|---|---|--|-------------------------------|----------------------------|-----------------------|---------------------|--|---|-----------------------|---------------------|----------------------|-------------------------------|----------------------------|--------------------|-----------------------|----------------------|---------------------------|--|---------------------------|--|--|
| Coumpound | | N-CADHERIN; CHAIN: A; | COAGULATION FACTOR | VIIA (LIGHT CHAIN); CHAIN: | L; COAGULATION FACTOR | VIIA (HEAVY CHAIN); | CHAIN: H; INFER IID IL INHIBITOR; CHAIN: C; | COAGULATION FACTOR VITA (LIGHT CHAIN): CHAIN: | L; COAGULATION FACTOR | VIIA (HEAVY CHAIN); | INHIBITOR; CHAIN: C; | COAGULATION FACTOR | VIIA (LIGHT CHAIN); CHAIN: | VIIA CHEAVY CHAIN: | CHAIN: H: TRIPEPTIDYL | INHIBITOR; CHAIN: C; | EPITHELIAL CADHERIN; | CHAIN: NULL; | EPITHELIAL CADHERIN; | CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; |
| SeqFold | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF score | | 0.21 | 0.36 | 96.0 | | _ | 0.88 | _ | 0.57 | | | | | -0.08 | | | | -0.15 | | | | | 0.13 | | 0.27 | | 0.45 |
| Verify | | -0.28 | 80.0 | 95.0 | -0.13 | 65.0 | 0.35 | 0.48 | 89.0 | | | | | 10.0 | | | | 80.0 | | | | | 0.33 | | 0.24 | | 0.04 |
| PSI- BLAST | | 1.10E-59 | 1.80E-35 | 7.20E-28 | 1.80E-25 | 1.10E-63 | 1.80E-34 | 3.60E-34 | 1.20E-21 | | | | | 3.60E-13 | | | | 7.20E-11 | | | | | 7.20E-08 | | 7.80E-20 | | 1238 1.30E-17 |
| End AA | | 248 | 926 | 799 | 812 | 216 | 1022 | 1129 | 3947 | | | | | 9268 | | | | 4168 | _ | | | | 1133 | | 1133 | | 1238 |
| Start AA | | 39 | 390 | 467 | 573 | 717 | 827 | 932 | 3865 | | | | | 3904 | | | | 4082 | _ | | | | 1026 | | 1041 | | 1145 |
| Chain ID | | ∢ | ¥ | Ą | A | ٧ | ¥ | ¥ | T | | | | | J | | | | J | | | | | | | | | |
| PDB DD | | Ing | Incj | Incj | Incj | Incj | Incj | Incj | lqfk | | | | | 19fk | | | | 뇶 | | | | | Isuh | | lsvh | | lsnh |
| SEQ NO: | | 608 | 608 | 809 | 608 | 608 | 608 | 608 | 608 | | | | | 608 | | | | 608 | | | | | 6 6 | | 608 | | 608 |

| PDB annotation | ADHESION | KIN; CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | IN; CELL ADHESION UVOMORULIN; | CADHERIN, CALCIUM BINDING, CELL ADHESION | Ī | CADHERIN, CALCIUM BINDING, CELL ADHESION | KIN; CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL. | ADHESION | | KIN; CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | Ī | CADHERIN, CALCIUM BINDING, CELL ADHESION | Ī | CADHERIN, CALCIUM BINDING, CELL ADHESION | | CADHERIN, CALCIUM BINDING, CELL ADHESION | VIN; CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL | Ī | CADHERIN, CALCIUM BINDING, CELL ADHESION | Ī | CADHERIN, CALCIUM BINDING, CELL ADHESION | r | CADHERIN, CALCIUM BINDING, CELL ADHESION | ĺ |
|------------------|----------|---|-------------------------------|--|----------------------|--|---|----------|--------------------------------------|---|----------------------|--|----------------------|--|----------------------|--|---|----------------------|--|----------------------|--|----------------------|--|-------------------|
| Coumpound | | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; | CHAIN: NULL; | EPITHELIAL CADHERIN; | CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL: | | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; | CHAIN: NULL; | EPITHELIAL CADHERIN; | CHAIN: NULL; | EPITHELIAL CADHERIN; | CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; | CHAIN: NULL; | EPITHELIAL CADHERIN; | CHAIN: NULL; | EPITHELIAL CADHERIN; | CHAIN: NULL; | Commertal Canmon. |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 6.4 | 0.62 | | 0.25 | | 0.63 | | 0.11 | 0.07 | 0.31 | | 60.0 | , | 89.0 | | 99.0 | 0.48 | | 0.39 | | 0.13 | | 910 |
| Verify | | -0.03 | 0.54 | | 0.3 | | 0.45 | | 0.14 | 0.35 | 0.41 | | 0.2 | | 0.07 | | 90:00 | -0.06 | | -0.24 | | -0.41 | | 5 |
| PSI- BLAST | | 7.20E-08 | 1.30E-10 | | 1444 1.80E-21 | | 1.30E-08 | | 1551 5.40E-07 | 2.60E-07 | 1650 1.00E-12 | | 1.40E-08 | | 1.30E-12 | | 3.60E-06 | 1.30E-14 | | 3.60E-05 | | 5.40E-07 | | 1 KOE-05 |
| End | | 1238 | 1334 | | 1444 | | 1549 | | 1551 | 226 | 1650 | | 1656 | | 1754 | | 1754 | 1867 | | 1868 | | 252 | | 1964 |
| Start AA | | 1711 | 1249 | | 1350 | | 1455 | | 1455 | 155 | 1570 | | 1589 | | 1991 | | 1690 | 1771 | | 1780 | | 182 | | 1808 |
| Chain | | | | | | | | | | | | | | | | | | | | | | | | |
| 80 a | | 1suh | Isuh | | 1suh | | 1suh | | Isuh | 1suh | Isuh | | 1suh | | 1suh | | 1suh | Isuh | | Isuh | | Isuh | | 1suh |
| SEQ NO: | | 608 | 808 | | 809 | | 608 | Ī | 809 | 809 | 809 | | 809 | | 809 | | 608 | 608 | | 608 | | 809 | | 608 |

| | r— | | | | | | | | | | | | | т |
|------------------|--|--|--|--|--|--|--|--|--|--|--|--|--|--|
| PDB annotation | CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN: CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION |
| Coumpound | CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELJAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; |
| SeqFold score | | | | | | | | | | | | | | |
| PMF | | 1202.08 | 60:00 | 0.12 | 0.57 | 0.46 | 0.77 | 0.94 | 0.58 | 90:0 | 0.03 | 86:0 | 0.12 | 66:0 |
| Verify score | | 0.17 | 0.42 | 0.05 | -0.23 | -0.36 | 0.44 | 0.4 | 0.03 | -0.37 | -0.2 | 0.16 | 0.02 | 0.51 |
| PSI- BLAST | | 7.20E-18 | 2.60E-15 | 3.60E-07 | 1.30E-14 | 3.60E-10 | 3.90E-20 | 2375 1.10E-08 | 3.90E-05 | | 3.60E-12 | 1.306-13 | 2.60E-10 | 1.40E-23 |
| End | | 5066 | 2163 | 2167 | 2268 | 2268 | 2375 | 2375 | 2475 | | 2581 | 2581 | 7681 | 2793 |
| Start AA | | 2761 | 2084 | 2104 | 2178 | 2178 | 2280 | 2306 | 2395 | 2414 | 2488 | 2489 | 2591 | 2692 |
| Chain D | | | | | | | | | | | | | | |
| PDB UD | | lsuh . | Isuh | Isuh | lsuh | 1suh | Isuh | lsuĥ | Isuh | Isuh | lsuh | lsuh | Isuh | 1suh |
| SEQ Sign | | 608 | 808 | 608 | 809 | 608 | 808 | 608 | 608 | 608 | 808 | 809 | 608 | 608 |

| PDB annotation | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UYOMORULIN: CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING; CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN. CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL |
|------------------|--|--|--|--|--|--|--|--|--|--|--|--|--|--|
| Coumpound | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELJAL CADHERIN; CHAIN: NULL: | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; |
| SeqFold score | | | | | | | | | | | | | | |
| PMF | 0.87 | 0.53 | 0.93 | 0.86 | 0.89 | 0.55 | 0.25 | 0.82 | 86:0 | 0.94 | 0.65 | 0.24 | 0.3 | 0.19 |
| Verify | 0.43 | -0.01 | 0.37 | -0.07 | 0.36 | 0.33 | 0.43 | 9.6 | 0.58 | 9.0 | 0.56 | 0.08 | -0.21 | -0.03 |
| PSI- BLAST | 2.60E-21 | I.40E-08 | 1.20E-14 | 1.80E-05 | 2.60E-21 | 3.60E-06 | 3.90E-12 | 1.30E-13 | 3.90E-21 | 5.40E-05 | 6.50E-11 | 0.0001 | 9.00E-06 | 1.30E-15 |
| End AA | 2902 | 2902 | 3007 | 3007 | 3109 | 3109 | 3213 | 3317 | 3422 | 3422 | 3524 | 454 | 454 | 560 |
| Start | 2806 | 2831 | 2914 | 2941 | 3026 | 3045 | 3120 | 3225 | 3330 | 3355 | 3435 | 363 | 401 | 467 |
| Chain | | | | | | | | | | | | | | |
| PDB CD | 1suh | 1suh | 1sth | Isuh | Isuh | Isuh | 1suh | . Isuh | Isuh | Isuh | Isuh | Isuh | Isuh | Isuh |
| SEQ No. | 809 | 809 | 808 | 808 | 608 | 809 | 608 | 808 | 809 | 608 | 608 | 608 | 608 | 608 |

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| PDB annotation | ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | PLASMINOGEN ACTIVATION | BLOOD COAGULATION FACTOR STUART FACTOR, BLOOD COAGULATION FACTOR, SERINE PROTEINASE, EPIDERMAL 2 GROWTH FACTOR LIKE DOMAIN | | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 3, ECAD12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN, CALCIUM | CELL ADHESION PROTEIN EPITHELALL CADHERIN DOMAINS I AND 2, ECADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN |
|-----------------|----------|--|--|--|--|--|--|--|--|---|--|--|
| Coumpound | | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | T-PLASMINOGEN ACTIVATOR FI-G; ITPG 7 CHAIN: NULL: ITPG 8 | BLOOD COAGULATION FACTOR XA; CHAIN: L, C; | LECTIN (AGGLUTININ) WHEAT GERM AGGLUTININ (ISOLECTIN 2) 9 WGA 3 | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; |
| SeqFold | | | | | | | | | | | | |
| PMF | | 0.57 | 0.95 | 0.72 | 0.47 | 0.57 | 0.18 | 0.59 | 0.1 | -0.2 | 0.25 | 0.16 |
| Verify score | | 0.39 | -0.21 | 0.4 | 0.27 | 0.37 | 0.2 | 0.21 | -0.26 | 0.02 | -0.26 | 0.35 |
| PSI- BLAST | | 3.90E-05 | 7.20E-25 | 1.00E-17 | 1.30E-07 | 5.20E-13 | 9.00E-07 | 1.30E-18 | 7.20E-11 | 5,40E-12 | 3.60E-24 | 1.80E-17 |
| End | | 859 | 918 | 921 | 126 | 1026 | 1026 | 3940 | 3994 | 4234 | 370 | 145 |
| Start | | 280 | 716 | 826 | 854 | 026 | 656 | 3863 | 3904 | 4069 | 190 | 23 |
| Chain | | | | | | | | | 1 | A | A | ٧ |
| E E | | Isuh | Isuh | Isuh | Isuh | Isuh | Isuh | Itpg | Ixka | 9wga | 1edh | ledh |
| S B S | | 809 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 608 | 811 | 811 |

| | | | | | | | | | | | | | | _ | |
|------------------|--|---|---|---|---|---|---|---|---|---|---|---|---|---|----------------------------|
| PDB annotation | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DONAINS I AND 2, ECADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECAD 12, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN, | CELL ADHESION PROTEIN EPTHELIAL CADHERIN DONAINS I AND 2, ECADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN EPITHELIAL CADHERIN DOMAINS I AND 2, ECADIT, CADHERIN, CELL ADHESION PROTEIN, CALCIUM BINDING PROTEIN | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCG 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CADHERIN INCI 13 | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION PROTEIN CELL |
| Coumpound | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | E-CADHERIN; CHAIN: A, B; | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCG 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; INCI 3 | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN; CHAIN: A; | N-CADHERIN: CHAIN: A; | N-CADHERIN; CHAIN: A; |
| SeqFold score | | | | 124.11 | | | | | | | | | | | |
| PMF | 0.82 | _ | _ | | 0.03 | 0.63 | _ | 0.12 | 0.62 | 1 | 86.0 | 0.59 | 0.58 | 66.0 | _ |
| Verify score | 021 | 0.21 | 19:0 | | 0.07 | 0.34 | 0.16 | -0.15 | 0.44 | 0.35 | 0.21 | 0.31 | 0.31 | 0.24 | 0.29 |
| PSI- BLAST | 1.80E-30 | 7.20E-26 | 1.80E-51 | 1.80E-51 | 0.00018 | 1.80E-06 | 1.60E-19 | 0.00036 | 3.60E-07 | 5.40E-19 | 1.10E-26 | 3.60E-20 | 1.80E-31 | 7.20E-28 | 1.80E-55 |
| End | 474 | 584 | 237 | 254 | 238 | 473 | 143 | 238 | 474 | 145 | 370 | 145 | 474 | 999 | 238 |
| Start AA | 296 | 410 | 20 | 20 | 881 | 408 | 48 | 189 | 409 | 48 | 091 | 24 | 271 | 402 | 49 |
| Chain | Ą | ∢ | ¥ | ¥ | | | | В | В | В | A | ٧ | ٧ | A | ٧ |
| 808 OI | ledh | ledh | ledh | ledh | Jucg | lncg | Incg | Inci | lnci | Inci | Incj | Incj | Incj | lncj | Incj |
| SEQ B B S | 811 | 811 | 811 | 811 | 811 | 811 | 118 | 811 | 811 | 811 | 811 | 811 | 811 | 811 | 811 |

| | _ | | | | | | | | | | | | |
|------------------|------------------|---|--|--|---|---|--|--|--|--|---|---|---|
| PDB annotation | ADHESION PROTEIN | CELL ADHESION PROTEIN CELL ADHESION PROTEIN | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULN: CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN: CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | CELL ADHESION UVOMORULIN; CADHERIN, CALCIUM BINDING, CELL ADHESION | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERODNA) |
| Coumpound | | N-CADHERIN; CHAIN: A; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | EPITHELIAL CADHERIN; CHAIN: NULL; | QGSR ZINC FINGER PEPTIDE, CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C. | QGSK ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B. C: | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; |
| SeqFold score | | 125.8 | | | | | | | | | | | |
| PMF | | | 0.18 | 0.23 | 0.01 | 0.46 | 0.89 | | 1 | 0.1 | _ | 0.92 | - |
| Verify score | | | 0.22 | -0.08 | 0.36 | 0.3 | -0.15 | 9.65 | 0.58 | 0.23 | 19:0 | 89.0 | 0.34 |
| PSI- BLAST | | 1.80E-55 | 1.20E-16 | 0.0041 | 5.20E-12 | 1.30E-17 | 1.60E-08 | 9.00E-23 | 2.60E-29 | 1.00E-08 | 2.60E-35 | 3.60E-27 | 7.20E-49 |
| End | | 253 | 258 | 237 | 371 | 478 | 478 | 149 | 149 | 584 | 142 | 142 | 198 |
| Start AA | | 49 | 162 | 190 | 268 | 383 | 410 | 48 | 49 | 490 | 62 | 69 | 117 |
| Chain ID | | A | | | | | | | | | ٧ | Y | ပ |
| PDB CD | | Incj | Isuh | 1suh | lsuh | Isuh | Isuh | lsuh | 1suh | 1suh | Ialh | lalh | Jme y |
| S e S | | 811 | 811 | 811 | 811 | 811 | 811 | 118 | 811 | 811 | 813 | 813 | 813 |

| | | | | | | | , | |
|-----------------|--|--|---|--|--|--|---|---|
| PDB annotation | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERODNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | |
| Coumpound | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN; A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | TRANSCRIPTION REGULATION YEAST TRANSCRIPTION PACTOR ADRI (RESIDUES 130 - 159) IPAA 3 (PAPA - CARBOXY TERMINAL ZINC FINGER |
| SeqFold | , | | | 111.37 | | | | |
| PMF | _ | - · | _ | | _ | - | - | 0.34 |
| Verify score | 0.51 | 0.32 | 0.34 | | 0.27 | 0.63 | 0.39 | 0.13 |
| PSI- BLAST | 5.40E-50 | 1.80E-49 | 1.30E-49 | 1.30E-49 | 1.30E-49 | 9.00E-43 | 1.10E-48 | 9.00E-05 |
| End | 226 | 254 | 282 | 283 | 310 | 142 | 170 | 312 |
| Start | 145 | 173 | 201 | 201 | 229 | 89 | 68 | 286 |
| Chain | U | ပ | ပ | υ. | o · | ၁ | U | |
| PDB CI | J me | J me | Jme y | Ime y | lme y | Jme y | J me | l paa |
| SE B SE | 813 | 813 | 813 | 813 | 813 | 813 | 813 | 813 |

| PDB annotation | | ZINC FINGER TRANSCRIPTION FACTOR SPI; ZINC FINGER, TRANSCRIPTION ACTIVATION SPI | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION) REGULATION/DNA), RNA REGULATION/DNA), RNA ROLYMERSASE III, 2 TRANSCRIPTION NUTLATION ZNC PRINCER PROCESS | COMPLEX (TRANSCAPTION REGULATION/DNA) COMPLEX (TRANSCAPTION REGULATION/DNA), RNA REGULATION/DNA), RNA ROLYMERSES BIL 2 TRANSCAPTION NUTLATION 2 NA FRANSCAPTION NUTLATION 2 NA FRANSCAPTION | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA REGULATION/DNA), RNA POLYMERASE BIL 2 TRANSCRIPTION NUTLATION 2NG PROGREP PROGREP | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION) REGULATION/DNA), RNA REGULATION/DNA), RNA POLYMBERSE III, 2 TRANSCRIPTION INITIATION ZINC, PROGRE PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-YANG I; TRANSCRIPTION INITIATION, INITIATIOR ELEMENT, YYI, ZINC 2 FUNGER PROTEIN DIAN-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX |
|----------------|---|---|---|---|--|--|--|
| Coumpound | DOMAIN) MUTANT WITH THA 4 RRO 131 REPLACED BY ALA, PRO 133 REPLACED BY ALA, CYS 140 IPAA 5 REPLACED BY ALA (P131A,P133A,C140A) (NR, | SPIF2; CHAIN: NULL; | TFIIIA, CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAN: A, D; 58 RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | YYI; CHAIN: C; ADENO- SASCIA/TED VIRUS PS INITACIA: ELEMENT DNA; CHAIN: A, B; |
| SeqFold | | | | 111.05 | | | |
| PMF | | 0.35 | 0.98 | | 1- | 1 | - |
| Verify | | 0.27 | 0.17 | | 0.36 | 0.38 | 0.26 |
| PSI- BLAST | | 5.40E-07 | 1.80E-38 | 2.60E-61 | 9.00E-36 | 7.20E-37 | 2.60E-49 |
| End | | 312 | 270 | 310 | 312 | 235 | 254 |
| Start AA | | 286 | 118 | 145 | 174 | 06 | 144 |
| Chain ID | | | ٧ | ∢ | ¥. | < | ၁ |
| PDB ID | | 1sp2 | 1116 | 146 | 9#1 | 1116 | Jubd |
| SEQ NO: | | 813 | 813 | 813 | 813 | 813 | 813 |

| PDB annotation | COMPLEX (TRANSCRIPTION REGULATIONDAN) YING-YAN I; TRANSCRIPTON INITIATION INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDAN) | COMPLEX (TRANSCRIPTION REGULATIONONA) YING-YANO 1; TRANSCRIPTION INITIATION, INITIATIOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, JUA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULT/TON/DANA) TING-YAN 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATIONDAN) TING-YAND 1; TRANSCRIPTION INITIATION INITIATIOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN JUA-PROTEIN RECOGNITION, I COMPLEX (TRANSCRIPTION REGULATIONA) | COMPLEX (TRANSCRIPTION REGULATIONDAN) YING-YAND I; TRANSCRIPTION INITIATION, INITIATIOR ELEMENT, YYI, ZINO Z FINGER PROTEIN, DNA-PROTEIN REGORDITION, 3 COMPLEX TRANSCRIPTION REGULATIONDAN | COMPLEX (TRANSCRIPTION REGULATIONONA) YING-YANG I; TRANSCRIPTION INTIA/TION, INITIA/TOR ELEMENT, YY1, ZINC 2 FINGER ROTEN, DIAA-ROTEIN RECOGNITION, 3 COMPLEX |
|-----------------|--|---|--|---|---|---|
| Coumpound | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS CHAIN: A, B; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YY; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; |
| SeqFold | * | 105.14 | | | | |
| PMF | - | | _ | - | 0.94 | 0.98 |
| Verify score | 0.25 | | 0.03 | 0.37 | 0.49 | 0.34 |
| PSI- BLAST | 3.60E-35 | 1.30E-50 | 7.80E-50 | 1.30E-50 | 2.60E-43 | 1.80E-33 |
| End AA | 254 | 283 | 283 | 310 | 170 | 071 |
| Start | 153 | 172 | | 199 | 99 | 69 |
| Chain ID | ပ | ပ | ວ | υ | ပ | U |
| E CO | Jubd | lubd | 1ubd | lubd | 1ubd | Inbd |
| S e S | 813 | 813 | 813 | 813 | 813 | 813 |

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|------------------|--------------------------------|--|--------------------------------|-----------------------------|---|---------------------------|---|---------------------------|------------------------------------|----------------------|---------------------------|------------------------------------|--|---------------------------|------------------------------------|----------------------------|---|---------------------------|---------------------------|----------------------|---------------------------|------------------------------------|---|---------------------------|------------------------------------|----------------------------|----------------------|---------------------------|------------------------------------|--|---|-------------------------|
| PDB annotation | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-YANG I; TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGIT ATTION/DNA) | TRANSCRIPTION REGILIATION | TRANSCRIPTION REGULATION, ADR1. ZINC FINGER, NMR | COMPLEX (DNA-BINDING · | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | ZINC FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | ZINC BINGED COMPLEY (DNA) | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | ZINC FINGER, COMPLEX (DNA- BINDING PROTFINONA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI, | ZINC FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-FINGER GLI; GLI. | ZINC FINGER, COMPLEX (DNA- BINDING PROTFIN/DNA) | 6 | TRANSFERASE SAM-BINDING |
| Coumpound | | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | ADRI: CHAIN: NIII.I. | | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, | aî. | ZINC FINGER PROTEIN GLII; | CHAIN: A: DNA; CHAIN: C, | ÷, | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, | ä | 100000000000000000000000000000000000000 | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, | î | ZINC FINGER PROTEIN GLI1; | CHAIN: A; DNA; CHAIN: C, | 'n | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, | Ö | | ZINC FINGER PROTEIN GLI1; | CHAIN: A; DNA; CHAIN: C, | ä | | HNRNP ARGININE N- |
| SeqFold score | | | | | | | | 107.01 | _ | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | _ | | | | _ | | | | | 86.0 | | | _ | | | | _ | | | _ | | | - | | | | 95 | | | | 0.34 |
| Verify score | | 0.62 | | | | 0.74 | | | | | 0.23 | | | 0.39 | | | | 0.41 | | | 0.42 | | | 0.4 | | | | 0.45 | | | | -0.02 |
| PSI- BLAST | | 1.80E-34 | | | | 2.60E-23 | | 3.90E-62 | | | 3.90E-62 | | | 5.40E-34 | | | ** 0000 | 3.90E-43 | | | 1.30E-30 | | | 9.10E-60 | | | | 1.80E-33 | | | | 9.00E-58 |
| End | | 861 | | | | 911 | | 284 | | | 312 | | | 309 | | | | 172 | | | 691 | | | 256 | | | | 222 | | | | 288 |
| Start | | 26 | | | | 62 | | 145 | | • | 145 | | | 181 | | | | 62 | | | 73 | | | 68 | | | | 26 | | | | 2 |
| Chain ID | | ပ | | | | | | Ą | | | ٧ | | | Ą | | | | ٧ | | | Ą | | | V | | | | ∢ | | | | _ |
| PDB CI | | lubd | | | | 2adr | | 2gli | | | 2gli | _ | | 2gli | | | | Zgli | | | 2gli | | | 2gli | _ | | | 2gli | | | | 1 <u>g</u> 69 |
| S e S | | 813 | | | | 813 | | 813 | | | 813 | | | 813 | | | | 513 | | | 813 | | | 813 | | | | 813 | | | | 814 |

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|-----------------|--|--|---|---|---|-------------------|----------------------------|--------------------------|--------------------------|---------------------------------|---------------------------------------|-------------------|----------------------------|--------------------------|--------------------------|------------------------|-----------------------|--|---|-----------------------------|----------------------------|-----------------------|--------------|---|-------------------------------|
| PDB annotation | DOMAIN, BETA-BARREL, MIXED ALPHA-BETA, HEXAMER, 2 DIMER | SCAFFOLD PROTEIN SCAFFOLD PROTEIN, PP2A, PHOSPHORYLATION, HEAT REPEAT. | TOXIN BINDING PROTEIN TWO DOMAINS: BETA PROPELLER AND ALPHA/BETA FOLD | TRANSCRIPTION INHIBITOR BETA- PROPELLER | TRANSCRIPTION INHIBITOR BETA- PROPELLER | COMPLEX (GTP- | BINDING/TRANSDUCER) BETAI, | TRANSDUCIN BETA SUBUNIT; | STIBLINIT: COMPLEX (GTP- | BINDING/TRANSDUCER), G PROTEIN, | HETEROTRIMER 2 SIGNAL TRANSDUCTION | COMPLEX (GTP- | BINDING/TRANSDUCER) BETA1, | TRANSDUCIN BETA SUBUNIT; | GAMMAI, TRANSDUCIN GAMMA | SUBUNIT; COMPLEX (GIP- | HETEROTRIMER 2 SIGNAL | TRANSDUCTION | NUCLEAR TRANSPORT PROTEIN COMPLEX HEAT REPEATS NITCLEAR | TRANSPORT PROTEIN COMPLEX | ARMADILLO REPEAT ARMADILLO | REPEAT, BETA-CATENIN, | CYTOSKELETON | COMPLEX (HSP24/HSP70) HSP70, GRPE, MOLECULAR CHAPFRONE | NUCLEOTIDE EXCHANGE 2 FACTOR, |
| Coumpound | METHYLTRANSFERASE; CHAIN: 1, 2, 3, 4, 5, 6; | PROTEIN PHOSPHATASE PP2A; CHAIN: A, B; | TOLB PROTEIN; CHAIN: A; | TRANSCRIPTIONAL REPRESSOR TUPI; CHAIN: A, B, C; | TRANSCRIPTIONAL REPRESSOR TUPI; CHAIN: A, B, C; | GT-ALPHA/GI-ALPHA | CHIMERA; CHAIN: A; GT- | BETA; CHAIN: B; GT- | CAMINIA, CHAIN: G, | | | GT-ALPHA/GI-ALPHA | CHIMERA; CHAIN: A; GT- | BETA; CHAIN: B; GT- | GAMMA; CHAIN: G; | | | - man of 7 or occording 5 or 5 or 5 or 5 or 5 or 5 or 5 or 5 o | KARYOPHERIN BETA2; | circuit p, ton', circuit c, | BETA-CATENIN; CHAIN: | NULL; | | NUCLEOTIDE EXCHANGE FACTOR GRPE: CHAIN: A. B. | MOLECULAR CHAPERONE |
| SeqFold | | | | | | | | | | | | | | | | | | | | | | | | 78.03 | |
| PMF | | 0.98 | 0.03 | - | _ | - | | | | | | - | | | | | | | 0.07 | | 0.23 | | | | |
| Verify score | | 0.32 | 0.16 | 0.12 | 0.28 | 0.18 | | | | | | 0.63 | | | | | | , | 9 | | -0.02 | | | | |
| PSI- BLAST | | 1.20E-07 | 0.0036 | 3.60E-60 | 3.60E-68 | 3.60E-60 | | | | | | 3.60E-73 | | | | | | 0000 | 5.20E-05 | | 2.60E-15 | | | 5.20E-41 | |
| End | | 520 | 1078 | 1099 | 1147 | 1096 | | | | | | 1144 | | | | | | 100 | 653 | | 653 | | | 222 | |
| Start AA | | 235 | 821 | 796 | 831 | 758 | | | | | | 823 | | | | | | 95 | 8 | | 345 | | | 51 | |
| Chain ED | | V | ٧ | ٧ | ٧ | В | | | | | | В | | | | | | | n | | | | | ¥ | |
| 90 0 | | 1b3u | lerz | lerj. | lerj | Igot | , | | | | | lgot | | | | | | | <u>ğ</u> | | 3pct | | | ldkg | |
| S e S | | 817 | 817 | 817 | 817 | 817 | | | | | | 817 | | | | | | ; | ž | | 817 | | I | 818 | |

| PDB annotation | COILED-COIL, COMPLEX (HSP24/HSP70) | COMPLEX (HSP24/HSP70) HSP70, GRPE, MOLECULAR CHAPERONE, NUCLEOTIDE EXCHANGE 2 FACTOR, COLLED-COIL, COMPLEX (HSP24/HSP70) | COMPLEX (HSP24/HSP70) HSP70, GRPE, MOLECULAR CHAPERONE, NUCLEOTIDE EXCHANGE 2 FACTOR, COLLED-COIL, COMPLEX (HSP24/HSP70) | COMPLEX (DNA-BRUDING PROTEIN; MAX, BNOTEIN) MAX, BND BINDING, BASIC-HELIX-LOOP-HELIX-LOOP-HELIX-LOOP-TRANSCRIPTION FACTOR, COMPLEX (DNA-BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN; MAX, PROTEIN) MAX BROTEIN; MAX, DNA BINDING, BASIC-HELIX-LOOP—HELIX-LEUCINE ZIPPER, 2 TRANOSERTION FACTOR, COMPLEX (DNA-BINDING PROTEINDING). | COMPLEX (TRANSCRIPTION FACTOR MAX/DNA) TRANSCRIPTIONAL REGULATION, DNA BINDING, COMPLEX 2 (TRANSCRIPTION FACTOR MAX/DNA) | COMPLEX (TRANSCRIPTION FACTOR | MAX/DNA) TRANSCRIPTIONAL | REGULATION, DNA BINDING, | FACTOR MAX/DNA) | | SCAFFOLD PROTEIN SCAFFOLD PROTEIN, PP2A, PHOSPHORYLATION, HEAT REPEAT | SMALL GTPASE KARYOPHERIN BETA, P95 SMALL GTPASE, NUCLEAR |
|---|------------------------------------|--|--|--|---|--|-------------------------------|----------------------------|--------------------------|-----------------|---|---|---|
| Coumpound | DNAK; CHAIN: D; | NUCLEOTIDE EXCHANGE FACTOR GRPE; CHAIN: A, B; MOLECULAR CHAPERONE DNAK; CHAIN: D; | NUCLEOTIDE EXCHANGE FACTOR GRPE; CHAIN: A, B; MOLECULAR CHAPERONE DNAK; CHAIN: D; | MAX PROTEIN; CHAIN: A, C; DNA; CHAIN: B, D; | MAX PROTEIN; CHAIN: A, C, DNA; CHAIN; B, D; | TRANSCRIPTION FACTOR MAX; CHAIN: A, B; DNA (5'- D(*CP*AP*CP*CP*GP*TP-3', CHAIN: C, D; | TRANSCRIPTION FACTOR | MAX; CHAIN: A, B; DNA (5'- | D(*CP*AP*CP*GP*GP*GP | D; | | PROTEIN PHOSPHATASE PP2A; CHAIN: A, B; | RAN; CHAIN: A, C; IMPORTIN BETA SUBUNIT; |
| SeqFold | | | | | | | | | | | | | |
| PMF | | 0.83 | 0.42 | 0.03 | 0.09 | 0 | 0.28 | | | | | _ | 0.82 |
| Verify score | | -0.15 | -0.29 | -0.73 | 8.0- | -0.58 | -0.27 | | | | | 0.55 | 0.25 |
| PSI- BLAST | | 1.80E-20 | 5.20E-41 | 3.60E-14 | 2.60E-13 | 1.60E-14 | 1.80E-14 | | | ļ | | 6.50E-08 | 0.0026 |
| End | | 221 | 220 | 203 | 219 | 203 | 203 | | | | | 373 | 235 |
| Start | | 53 | 19 | 135 | 140 | 131 | 132 | | | | | 44 | 131 |
| Chain | | ¥ | ∢ | ¥ | ∢ | V | В | | | | | A | В |
| 708 ID | | Idkg | ldkg | lan2 | lan2 | 1hlo | lhlo | | | | | 1b3u | libr |
| SEQ SO SO SO SO SO SO SO SO SO SO SO SO SO | | 818 | 818 | 820 | 820 | 820 | 820 | | | | 1 | 824 | 824 |

| PDB annotation | TRANSPORT RECEPTOR | SMALL GTPASE KAR YOPHERIN BETA, P95 SMALL GTPASE, NUCLEAR | TRANSPORT RECEPTOR | ARMADILLO REPEAT ARMADILLO | REPEAT, BETA-CATENIN, CYTOSKELETON | LYASE ACC SYNTHASE, S- | ADENOSYL-L-METHIONINE ETHYLENE BIOSYNTHESIS | RIFAMYCIN BIOSYNTHESIS (RIFD | GENE) AHBA SYNTHASE; RIFAMYCIN BIOSYNTHESIS (RIFD GENE) | TRANSFERASE TRANSFERASE. | METABOLIC ROLE, PYRIDOXAL 5'- | PHOSPHATE | AMINOTRANSFERASE | AMINOTRANSFERASE, PYRIDOXAL | ENZYME | TRANSFERASE AONS, 8-AMINO-7- | KETOPELARGONATE SYNTHASE; | PLP-DEPENDENT ACYL-COA | SYNTHASE, BIOTIN BIOSYNTHESIS, | 8-2 AMINO-7-OXONANOATE | SYNTHASE, 8-AMINO-7- | KETOPELARGONATE 3 SYNTHASE, TRANSFFRASE | LYASE ALPHA/BETA FOLD | TRANSFERASE SHMT; | HYDROXYMETHYL TRANSFERASE, 1 | CARBON METABOLISM | METHIONINE BIOS YNTHESIS BETA | CYSTATHIONASE; PLP-DEPENDENT | ENZYMES, METHIONINE | BIOSYNTHESIS, C-S BETA 2 LYASE | LYASE CGS; LYASE, LLP-DEPENDENT | ENZYMES, METHIONINE | TRANSEED ASE AMERICAN ASSESSMENT | FOLD, LARGE PLP-BINDING DOMAIN, |
|------------------|--------------------|--|--------------------|----------------------------|---------------------------------------|------------------------|---|------------------------------|--|--------------------------|-------------------------------|------------------|------------------|-----------------------------|--------------|------------------------------|---------------------------|------------------------|--------------------------------|------------------------|----------------------|--|-------------------------|-------------------|------------------------------|---------------------|-------------------------------|------------------------------|---------------------|--------------------------------|---------------------------------|---------------------------|----------------------------------|---------------------------------|
| Coumpound | CHAIN: B, D; | RAN; CHAIN: A, C; IMPORTIN BETA SUBUNIT; | CHAIN: B, D; | BETA-CATENIN; CHAIN: | NULL; | 1-AMINOCYCLOPROPANE-1- | CARBOXYLATE SYNTHASE; CHAIN: A, B; | 3-AMINO-5- | HYDROXYBENZOIC ACID SYNTHASE: CHAIN: A: | SERINE | HYDROXYMETHYLTRANSF | ERASE; CHAIN: A; | ASPARTATE | AMINOTRANSFERASE; | CHAIN: A, B; | 8-AMINO-7-OXONANOATE | SYNTHASE; CHAIN: A; | | | | | | CSDB PROTEIN: CHAIN: A: | SERINE | HYDROXYMETHYLTRANSF | ERASE; CHAIN: A, B; | CYSTATHIONINE BETA- | LYASE; CHAIN: A, B; | | | CYSTATHIONINE GAMMA- | SYNTHASE; CHAIN: A, B, C, | MALV BROTERI, CHARLA | MALT PROTEIN; CHAIN: A, B; |
| SeqFold score | | | | | | | | | | | | | | | | 52.33 | | | | | | | | | | | | | | | | | | |
| PMF | | 0.47 | | 0.99 | | 0.22 | | -0.13 | | 0 | | | | 1202.08 | | | | _ | | | | | _ | -1.41 | | | -0.19 | | | | -0.03 | | 0 61 | 100 |
| Verify score | | 90:0 | | 0.41 | | 0.41 | | 0.12 | | 0.25 | | | 0.29 | | | | | | | | | | 0.51 | 0.04 | | | 0.1 | | | | 0.2 | | 900 | 90.5 |
| PSI- BLAST | | 6.50E-06 | | 6.50E-14 | | 5.40E-14 | | 3.60E-37 | | 5.40E-50 | | | 1.80E-52 | | | 7.20E-06 | | | | | | | 9.00E-57 | 3.60E-51 | | | 3.60E-16 | | | | 5.40E-34 | | 1 805 00 | 1.005-09 |
| End | | 303 | | 404 | | 294 | | 317 | | 312 | | | 309 | | | 317 | | | | | | | 311 | 312 | | | 314 | | | | 313 | | 250 | 63 |
| Start AA | | 201 | | 154 | | 2 | | - 26 | | _ | | | 3 | | | _ | | | | | | | 01 | _ | | | 93 | | | | 22 | | 135 | 3 |
| Chain ID | | В | | | | ٧ | | ٧ | | Ą | | | A | | | ٧ | | | | | | | A | ٧ | | | Y | | | | ۷ | | • | |
| PDB UD | | libr | | 3pct | | 1b8g | | 169h | | 1bj4 | , | | 1bjw | | | 1bs0 | | | | | | | lc0n | 1cjo | | | Icli | | | | ls | | 1,43 | 1707 |
| SEQ NO: | | 824 | | 824 | | 826 | | 826 | | 826 | | | 826 | | | 826 | | | | | | | 826 | 826 | | | 826 | | | | 826 | | 826 | 020 |

| PDB annotation | SMALL C- 2 TERMINAL DOMAIN, OPEN ALPHA-BETA STRUCTURE, | TRANSFERASE SHMT, SERINE METHYLASE; ALPHA PLP ASPARTATE, AMINO TRANSFERASE, (AAT)-LIKE FOLD | TRANSFERASE PLP-DEPENDENT ENZYMES, IRON-SULFUR-CLUSTER SYNTHESIS, C-S 2 BETA LYASE | TRANSFEKASE SHMT; SERINE- GLYCINE CONVERSION, PYRIDOXAL S-PHOSPHATE, 2 TETRAHYDROFOLATE, ASYMMETRIC DIMER | LYASE METHIONINE BIOSYNTHESIS, PYRIDOXAL 5'-PHOSPHATE, GAMMA- 2 FAMILY, LYASE | | LYASE LYASE, PLP-DEPENDENT ENZYME, PYRIDOXAL PHOSPHATE | LIGASE E6AP; UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | LIGASE EGAP; UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | SH3 PROTOTYPE WWPROTOTYPE, PROTEIN DESIGN | SH3 PROTOTYPE WWPROTOTYPE, PROTEIN DESIGN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) |
|----------------|---|---|--|---|---|--|---|---|---|---|---|---|--|
| Coumpound | | SERINE HYDROXYMETHYLTRANSF ERASE; CHAIN: A, B, C, D; | AMINOTRANSFERASE; CHAIN: A, B; | SERINE HYDROXYMETHYLTRANSF ERASE; CHAIN: A, B, C, D; | CYSTATHIONINE GAMMA- SYNTHASE; CHAIN: A, B, C, D, E, F, G, H; | LYASE(CARBON-CARBON) TYROSINE PHENOL-LYASE (E.C.4.1.99.2) ITPL 3 | TYROSINE PHENOL-LYASE; CHAIN: A, B; | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2; CHAIN: D. | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2: CHAIN: D: | WWPROTOTYPE; CHAIN: A; | WWPROTOTYPE; CHAIN: A; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE | BINDING SITE; CHAIN: B, C; QGSR ZINC FINGER |
| SeqFold | | - | | | | | | 217.98 | | | | | |
| PMF | | 0.17 | _ | -1.41 | -0.06 | -0.03 | -0.06 | | _ | 0.29 | 0.35 | 0.24 | 1-1 |
| Verify | | -0.07 | 0.62 | 0.09 | 0.19 | 0.21 | 0.02 | | 0.38 | 90:0 | 10.0 | -0.37 | 0.04 |
| PSI. BLAST | | 9.00E-54 | 3.60E-58 | 5.40E-50 | 7.20E-21 | 3.60E-09 | 1.30E-08 | 1.10E-45 | 1.10E-45 | 2.60E-11 | 3.90E-12 | 3.60E-26 | 2.60E-39 |
| End | | 314 | 317 | 312 | 311 | 311 | 311 | 1566 | 1565 | 841 | 1019 | 259 | 315 |
| Start | | ∞ | 32 | - | 20 | 101 | 101 | 1213 | 1239 | 608 | 982 | 179 | 235 |
| Chain ID | | ¥ | ¥ | ¥ | Ą | ¥ | 4 | ٧ | ∀ | ٧ | ۷ | 4 | A |
| PDB | | ojp! | leg5 | leji | lqgn | 귤 | 2tp1 | 1c4z | lc4z | лео в | 3 E | lalh | lalh |
| SEQ NO: | | 826 | | | | 928 | 826 | 830 | | 830 | 830 | 832 | 832 |

| | | | | | | | | _ | | |
|------------------|--|---|---|---|--|--|---|--|---|--------------------------------|
| PDB annotation | COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA PINTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZNC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC |
| Coumpound | PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B. C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | DNA, CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; |
| SeqFold score | | | | | | | | ļ | | |
| PMF | | _ | 66.0 | 0.98 | 70.0 | 0.52 | - | _ | _ | - |
| Verify | | 0.48 | 0.41 | 0.27 | -0.35 | -0.16 | 0.1 | 0.23 | 0.55 | 0.49 |
| PSI- BLAST | | 9.10E-38 | 1.40E-30 | 3.90E-39 | 3.60E-40 | 1.10E-43 | 3.60E-45 | 1.60E-46 | 1.40E-47 | 1.30E-48 |
| End A.A. | | 344 | 829 | 829 | 231 | | 287 | 315 | 343 | 371 |
| Start AA | | 263 | 598 | 298 | 150 | 178 | 506 | 234 | 262 | 290 |
| Chain Et | | ∀ | < | ٧ | ن ن | υ | ပ | ပ | O | U |
| 80 a | | lalh | laih | lalh | Jme y | Jme y | Jme y | J me | y Jme | Ime |
| S a S | | 832 | 832 | 832 | 832 | 832 | 832 | 832 | 832 | 832 |

| PDB annotation | FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERZDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA |
|------------------|---|--|---|---|--|---|--|--|---|
| Coumpound | CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN; A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN; C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER |
| SeqFold score | | | | | | | | | |
| PMF score | | _ | _ | _ | _ | _ | 96.0 | - | _ |
| Verify score | | 0.62 | 0.34 | 0.27 | 0.42 | 0.16 | -0.22 | 0.1 | 0.43 |
| PSI- BLAST | | 1.80E-49 | 1.40E-49 | 3.60E-50 | 5.40E-50 | 7.20E-50 | 6.50E-33 | 1.10E-49 | 7.20E-48 |
| End | | 399 | 427 | 455 | 483 | 511 | 538 | 539 | 594 |
| Start AA | | 318 | 346 | 374 | 402 | 430 | 430 | 458 | 514 |
| Chain ID | | ၁ | ပ | ၁ | ပ | ၁ | ე | ပ | ၁ |
| PDB ID | y | Ime y | lme y | Ime y | y Jine | Ime y | Jme y | Jme y | lme y |
| SEQ No: D | | 832 | 832 | 832 | 832 | 832 | 832 | 832 | 832 |

| | | | | | | | | | | _ | | | | _ | _ | | | _ | | | | | | | | _ | |
|-----------------|---|---|---|--------------------------------|--|--------------------------------|-----------------------|----------------------------|-------------------|--------------------------------|-----------------------|--------------------------------|----------------------------|--------------------------------|-----------------------|--------------------------------|-------------------|------------------------|----------------------------------|-------------------------------|---------------------------------|-------------------|--------------------------------|---|----------------------------|--------------------------------|--|
| PDB annotation | INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, FROIEM-DIAG INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC, FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | (ZINC FINGER/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) TFIIIA; 5S GENE; | TRANSCRIPTION FACTOR 5S RNA 2 | GENE, DNA BINDING PROTEIN, ZINC | FINGER, COMPLEX 3 | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGIT ATTOMONA) TELLA: 58 CENE: | NMR, TFIIIA, PROTEIN, DNA, | TRANSCRIPTION FACTOR, 5S RNA 2 | GENE, DNA BINDING PROTEIN, ZINC FINGER, COMPLEX 3 |
| Coumpound | PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; | PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, r, G; | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | DNA: CHAIN: A. B. D. E. | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | TRANSCRIPTION FACTOR | IIIA; CHAIN: A; 5S RNA | OENE; CHAIN: E, F; | | | | TRANSCRIPTION FACTOR | GENE, CHAIN: E, F; | | |
| SeqFold | | | | 101.87 | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | _ | | | | _ | | | | - | | | | 0.94 | | | | 0.99 | | | | | | 0 | | | |
| Verify score | | 69:0 | | | | 0.71 | | | | 0.39 | | | | 0.06 | | | | 0.15 | | | | | | 9.78 | | | |
| PSI- BLAST | | 1.80E-50 | | 1.80E-50 | | 3.60E-50 | | | | 1.80E-49 | | | | 1.30E-12 | ! | | | 1.40E-20 | | | | | | 3.60E-18 | | | |
| End | | 622 | | 623 | | 650 | | | | 829 | | | | 371 | | | | 511 | | | | | | 200 | | | |
| Start | | 541 | | 541 | | 695 | | | | 597 | | | | 344 | | | | 431 | | | | | | 487 | | | |
| Chain ID | | o | | ၁ | | ပ | | | | ပ | | | | c | | | | Ą | | | | | | ۷. | | | |
| PDB ED | | J. J. | | 1mc | ~ ~ | Ime | ^ | _ | | lme | > | | | Ime | ^ | _ | | 9 | | | | | | 9 | | | |
| S e S | | 832 | | 832 | | 832 | | | | 832 | | | | 832 | | | | 832 | | | | | | 832 | | | |

| PDB annotation | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX | (TRANSCRIPTION BEGIN ATTOMONA) DNA | POLYMERASE III. 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX | (IRANSCRIPTION | POLYMERASE III. 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX | (TRANSCRIPTION | REGULATION/DNA), RNA | POLYMERASE III, 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (IRANSCRIPTION | KEGULATION/DNA) COMPLEX | (IKANSCKIPTION | REGULATION/DNA), KNA | POLYMERASE III, 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | KEGULATION/DNA) COMPLEX | PEGIII ATIONONA) DNA | NEGOCIAL TOTAL STREET | NOTIMERADE III, 2 I RANSCRIPTION INTITATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX | (TRANSCRIPTION | REGULATION/DNA), RNA | POLYMERASE III, 2 TRANSCRIPTION | INITIATION, ZINC FINGER PROTEIN | COMPLEX (IKANSCKIPTION | TRANSCRIPTION COMPLEX | REGULATION/DNA), RNA |
|------------------|--------------------------------|--|------------------------------------|---------------------------------|---------------------------------|-------------------------|-------------------------|--------------------|---------------------------------|---------------------------------|-------------------------|-------------------------|--------------------|----------------------|---------------------------------|---------------------------------|-------------------------|-------------------------|--------------------|----------------------|---------------------------------|---------------------------------|-------------------------|-------------------------|----------------------|-----------------------|--|-------------------------|-------------------------|--------------------|----------------------|---------------------------------|---------------------------------|-------------------------|-----------------------|--|
| Coumpound | | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | | | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | | | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | | | 03 04 1 200 1 100000 | IFILIA; CHAIN: A, D; 3S | KIBOSOMAL KNA GENE; | CHAIN: B, C, E, F; | | | | TFIIIA; CHAIN: A, D; 5S | KIBOSOMAL KNA GENE; | CITATIV. B. C. E. I. | | | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; | CHAIN: B, C, E, F; | | | | IFILIA; CHAIN: A, D; 33 | CHAIN-B C F F. | (- to to to to to to to to to to to to to |
| SeqFold score | | | | | | 105.86 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.84 | | | | | | | | | _ | | | | | | -1.41 | | | | | | -1.41 | | | | | 0.89 | | | | | ò | 98.0 | | |
| Verify | | 60'0 | | | | | | | | | 0.15 | | | | | | 0.32 | | | | | | 91.0 | | | | | -0.05 | | | | | , | \$ | | |
| PSI- BLAST | | 1.80E-36 | | | | 1.30E-66 | | | | | I.60E-36 | | | | | 2000 | 3.60E-3/ | | | | | | 1,30E-36 | | | | | 1.60E-36 | | | | | 1 000 26 | 1.805-33 | | |
| End | | 352 | | | | 431 | | | | | 408 | | | | | | 404 | | | | | | 575 | | | | | 603 | | | | | | 63.1 | | |
| Start AA | | 202 | | | | 797 | | | | | 263 | | | | | 0.0 | 319 | | | | | 3 | 431 | | | | | 459 | | | | | 407 | 40 | | |
| Chain ID | | ٧ | | | | ٧ | | | | | V | | | | | | ∢ | | | | | | ٧ | | | | | Ą | | | | | | < | | |
| PDB ID | | 941 | 9 | | | 1116 | | | _ | | 9#1 | | | | | 2 | 8 | | | | | ŀ | 91 | | | | | 146 | | | | | 39. | 91 | | |
| SEQ NO: | | 832 | | | | 832 | | | | | 832 | | | | | 250 | 268 | | | | | 1 | 832 | | | | | 832 | | | _ | | 633 | 700 | | |

| . PDB annotation | POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX CTD ANSCRIPTION | REGULATION/DNA), RNA | INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION | TRANSCRIPTION INTERTION | INITIATOR ELEMENT, YYI, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG I; | IKANSCKIPIION INITIATION, | FINGER PROTEIN DNA-PROTEIN | RECOGNITION, 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | CTB ANSCRIPTION BEGIN ATTOMONA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | TECOGNITION, 3 COMPLEX | COMPLEX (TDANSCRIPTION | REGULATION/DNA) YING-YANG 1; | TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YY1, ZINC2 FINGER PROTEIN, DNA-PROTEIN |
|------------------|---|--|----------------------|---------------------------------|------------------------|-------------------------|--------------------------------|-----------------------------|--------------------------------|------------------------|------------------------------|---------------------------|----------------------------|------------------------|--------------------------------|------------------------|------------------------------|---------------------------|--------------------------------|-----------------------------|---------------------------------|------------------------|------------------------------|---------------------------|--------------------------------|-----------------------------|------------------------|------------------------|------------------------------|---------------------------|--|
| Coumpound | | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B. C. F. F. | CITALIN. D, C, E, F, | | YYI; CHAIN: C; ADENO- | ASSOCIATED VIRUS PS | CHAIN: A, B; | | | YYI; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | MINITALOR ELEMENT DNA; | CHAIN: A, B; | | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | VVI: CHAIN: C: ADENO. | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; | | | ONSIGN CHARLO: ANSIGN | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B; |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | - | | | 0.18 | | | | | 96.0 | | | | | | 69.0 | | | | | | 960 | ? | | | | | _ | | | |
| Verify | | 0.3 | | | -0.36 | | | | | -0.38 | | | | | | -0.37 | | | | | | -0.07 | | | | | | 0.01 | - | | |
| PSI- BLAST | | 7.20E-35 | | | 9.00E-29 | | | | | 3.60E-31 | | | | | | 1.30E-34 | | | | | | 2 60F-48 | 700.4 | | | | | 2 60E-22 | 1000 | | |
| End | | 099 | | | 259 | | | | | 287 | | | | | | 315 | | | | | | 371 | : | | | | | 343 | } | | |
| Start | | 515 | | | 158 | | | | | 186 | | | | | | 188 | | | | | | 233 | 1 | | | | | 242 | ! | | |
| Chain | | 4 | | | ပ | | | | | S | | | | | | C | | | | | | ر | , | | | | | |) | | |
| 10 E | | 911 | | | Pga- | | | | | 1ubd | | | | | | lubd | | | | | | Inhd | | | | | | 4.1 | } | | |
| S e S | | 832 | | | 832 | | | | | 832 | | | | | | 832 | | | | | | 832 | 3 | | | | | 833 | : | | |

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|------------------|--|---|---|---|--|---|--|
| PDB annotation | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATIONDAA) YING-YANG I; TRANSCRIPTION INITIATION, INITIATION ELEMENT YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX TRANSCRIPTION RECEIL AT ANY RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCREPTION REGULATIONDNA) YING-YANG I; TRANSCREPTON INTHATION, INTHATOR ELEMENT, YYI, ZINOZ FINGER PROTEIN, DNA-PROTEIN REGORNITON, 3 GOWELEX REGORNITON, 3 GOWELEX | COMPLEX (TRANSCRIPTION REGULATIONONA,) YING-YANG I; TRANSCRIPTION PURITATION, WITHATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRITTON REGULATIONONA) YING-YANG 1; TRANSCRIPTON PITATION, PITANSCRIPTON PITATION, PITANTOR ELEMENT, YYI, ZNO.2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITON, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATIONONA, YING-YANG I; TRANSCRIPTION MITHATION, MITHATOR ELEMENT YYI, ZINC2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG I; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YYI, ZINC 2 |
| Coumpound | | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A. B; | YY J; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INTIATOR ELEMENT DNA; CHAIN: A, B; | YY I; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; |
| SeqFold score | | | | | | | |
| PMF score | | | - | 0.88 | - | . 66.0 | - |
| Verify score | | 0.23 | 0.27 | 0.04 | 0.2 | -0.09 | -0.06 |
| PSI- BLAST | | 1.80E-34 | 5.40E-34 | 6.50E-52 | 3.60E-34 | 7.20E-36 | 1.40E-34 |
| End AA | | 371 | 399 | 483 | 455 | 483 | 511 |
| Start AA | | 270 | 298 | 344 | 354 | 382 | 410 |
| Chain | | ပ | U | ပ | υ · | ပ | ပ |
| PDB TD | | pqn | 1ubd | lubd | lubd | lubd | lubd |
| Se Se | | 832 | 832 | 832 | 832 | 832 | 832 |

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|------------------|---|--|---|---|-------------------------------|---|------------------------|---------------------------|--------------------------------|--|--------------------------------|------------------------|--|--------------------------------|-----------------------------|--|------------------------|------------------------------|-----------------------------|-----------------------------|------------------------|--------------------------------|---|---------------------------|
| PDB annotation | FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION, NITIATOR ELEMENT YY! 77NC? | FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; | INTITATOR ELEMENT, YY1, ZINC2 | FINGER PROTEIN, DNA-PROTEIN : RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGITI-ATION/DNA) | COMPLEX (TRANSCRIPTION | TRANSCRIPTION INITIATION. | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG I; | INITIATOR ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YANG 1; | INTIATOR ELEMENT: YYL ZINC2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG I; | TRANSCRIPTION INITIATION, |
| Coumpound | | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A. B. | | YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 | CHAIN: A, B; | | YY1; CHAIN: C; ADENO- | INITIATOR ELEMENT DNA: | CHAIN: A, B; | | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS PS INITIATOR RI EMENT DNA: | CHAIN: A, B; | | | YY1; CHAIN: C; ADENO- | ASSOCIATED VIRUS PS | CHAIN: A. B. | | | | AY1; CHAIN; C; ADENO- ASSOCIATED VIRUS PS | INITIATOR ELEMENT DNA; |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | 18.00 | 16.38 | |
| PMF | | 0.53 | | 0.34 | | | _ | | | | | _ | | | | | 96:0 | | | | | | | |
| Verify | | -0.42 | | 0.02 | | | 0.23 | | | | | 0.22 | | | | | 0.43 | | | | | | | |
| PSI- BLAST | | 3.90E-42 | | 3.60E-32 | | | 1.30E-47 | | | | | 5.40E-36 | | | | | 5.20E-51 | | | | | 1000 | 3.20E-51 | |
| End | | 594 | | 999 | | | 622 | | | | | 622 | | | | | 829 | | | | | Ġ. | 6/6 | |
| Start AA | | 428 | | 466 | | | 519 | | | | | 222 | | | | | 292 | | | | | | 8 | |
| Chain ID | | ပ | | υ υ | | | ပ | | | | | ပ | | | | | ပ | | | | | | د | |
| PDB ID | | pqnl | | Pdul | | | Jubd | | | | | P P | | | | | Iubd | | | | | 1 | pon I | |
| SEQ No: | | 832 | | 832 | | | 832 | | | | | 832 | | | | | 832 | | | | | 000 | 750 | |

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| PDB annotation | INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONIDNA) | COMPLEX (TRANSCRIPTION REQUILATION/DAY) YING-YANO I; TRANSCRIPTON INITIATION, INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTON REGULATION/DAY) | COMPLEX (TRANSCRIPTION REGIL-ATIONDANA) YING-YANG 1; TRANSCRIPTION INITIATION, INITIATIOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX TRANSCRIPTION REGIL ATIONNANA) | ZINC FINGER DNA BINDING DOMAIN DNA BINDING MOTIF, ZINC FINGER DNA BINDING DOMAIN | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) |
| Coumpound | CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YY I; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INTIATOR ELEMENT DNA; CHAIN: A, B; | SWIS; CHAIN: NULL, | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; |
| SeqFold | | | | | | | | | , |
| PMF | | - | 0.18 | 0.72 | 0.46 | 0.49 | _ | | 1 |
| Verify score | | -0.06 | 9.0 | 0.15 | -0.16 | -0.24 | -0.21 | -0.1 | 90:00 |
| PSI- BLAST | ١ | 5.40E-34 | 2.60E-06 | 0.00013 | 1.30E-36 | 1.60E-31 | 2.60E-52 | 5.20E-63 | 3.90E-64 |
| End | | 8/9 | 089 | 089 | 317 | 286 | 345 | 401 | 429 |
| Start | | 577 | 651 | 653 | 133 | 150 | 208 | 235 | 262 |
| Chain D | | ပ | ပ | | ¥ | A | Ą | ∢ | Y |
| PDB ID | | lubd | lubd | 1zfd | 2gli | 2gli | 2gli | 2gli | 2gli |
| SEQ B B S | | 832 | 832 | 832 | 832 | 832 | 832 | 832 | 832 |

| PDB annotation | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GIL; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FTVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI, GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | HYDROLASE HYDROLASE, | HALOALKANE DEHALOGENASE, ALPHA/BETA-HYDROLASE | HYDROLASE A/B HYDROLASE FOLD, |
|------------------|--|--|--|--|--|--|--|--|--|----------------------|--|-------------------------------|
| Coumpound | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLUI; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CḤAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | HALOALKANE | DEHALOGENASE; CHAIN: NULL; | HALOALKANE |
| SeqFold score | | | | | | | | | 91.33 | | | |
| PMF | _ | 6.0 | 0.19 | 66.0 | 0.49 | 0.19 | 66.0 | - | | 0.12 | | 0.21 |
| Verify score | 0.01 | 0.25 | -0.4 | 0.03 | -0.21 | -0.07 | -0.02 | 0.53 | | -0.1 | | -0.19 |
| PSI- BLAST | 3.60E-33 | 2.60E-64 | 3.90E-57 | 3.60E-34 | 1.10E-32 | 5.20E-60 | 5.40E-31 | 3.90E-64 | 3.90E-64 | 0.00078 | | 1332 0.0013 |
| End | 398 | 485 | 396 | 482 | \$65 | 652 | 624 | 829 | 089 | 1332 | | 1332 |
| Start | 270 | 318 | 346 | 354 | 438 | 459 | 494 | 541 | 241 | 1240 | | 1240 |
| Chain | ٧ | ٧ | Y | ٧ | ٧ | ٧ | ٧ | ¥ | < | | | ٧ |
| 108 10 | 2gli | 1b6g | | lcqw |
| Š e Š | 832 | 832 | 832 | 832 | 832 | 832 | 832 | 832 | 832 | 834 | | 834 |

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| PDB annotation | DEHALOGENASE I-S BOND | HYDROLASE TRIACYLGLYCEROL- HYDROLASE, X-RAY CRYSTALLOGRAPHY, 2 PSCUDOMONADACEAE, OXYANION, CIS-PEPTIDE. HYDROLASE | HYDROLASE ALPHA/BETA HYDROLASE, GLYCOPROTEIN | HYDROLASE TRIACYL-GLYCEROL LIPASE, LIPASE, ALPHA-BETA HYDROLASE FOLD, PSEUDOMONAS, PHOSPHONATE 2 INHIBITOR | | TRYPTOPHAN BIOSYNTHESIS TRYPTOPHAN INDOLE-IYAE; TRYPTOPHAN BIOSYNTHESIS; TRYPTOPHAN INDOLE-IYAE; PYRIDOXAL 2 5'-PHOSPHATE; | MONOVALENT CATION BINDING SITE | TRANSFERASE TRANSFERASE, METABOLIC ROLE, PYRIDOXAL 5'- PHOSPHATE | LYASE ALPHA/BETA FOLD | TRANSFERASE SHMT; HYDROXYMETHYL TRANSFERASE, 1 CARBON METABOLISM | LYASE CGS, LYASE, ILP-DEPENDENT ENZYMES, METHIONINE BIOSYNTHESIS | TRANSFERASE SHWT, SERINE METHYLASE; ALPHA PLP ASPARTATE, AMINO TRANSFERASE, (AATH-LIKE FOLD) | TRANSFERASE PLP-DEPENDENT ENZYMES, IRON-SULFUR-CLUSTER SYNTHESIS, C-S 2 BFTA I, YASE | TRANSFERASE PLP-DEPENDENT ENZYMES, IRON-SULFUR-CLUSTER SYNTHESIS, C-S 2 BETA LYASE |
| Coumpound | DEHALOGENASE; 1- CHLOROHEXANE CHAIN: A; | TRIACYLGLYČEROL HYDROLASE; CHAIN: NULL; | PALMITOYL PROTEIN THIOESTERASE 1: CHAIN: A: | LACTONIZNG LIPASE; CHAIN: A; | | TRYPTOPHAINASE; CHAIN: A, B, C, D; | | SERINE HYDROXYMETHYLTRANSF ERASE: CHAIN: A: | CSDB PROTEIN; CHAIN: A; | SERINE HYDROXYMETHYLTRANSF ERASE; CHAIN: A, B; | CYSTATHIONINE GAMMA- SYNTHASE, CHAIN: A, B, C, D: | SERINE HYDROXYMETHYLTRANSF ERASE; CHAIN: A, B, C, D; | AMINOTRANSFERASE; CHAIN: A, B: | AMINOTRANSFERASE; CHAIN: A, B; |
| SeqFold | | | | | | | | | | | | | | |
| PMF | | 69:0 | 0.53 | 0.46 | | 90:0 | | -0.07 | -1.41 | -0.13 | 0 | -1.41 | _ | _ |
| Verify score | | 40.0 | -0.1 | 0.13 | | 0.23 | | 0.08 | 80:0 | 0.05 | -0.28 | 0.17 | 0.22 | 0.1 |
| PSI- BLAST | | 0.00026 | 0.00026 | 0.00026 | | 5.40E-07 | | 7.20E-36 | 9.00E-41 | 7.20E-37 | 1.60E-31 | 3.60E-40 | 1.30E-50 | 1.80E-45 |
| End | | 1362 | 1362 | 1362 | | 241 | | 246 | 244 | 246 | 242 | 252 | 248 | 248 |
| Start | | 1251 | 1251 | 1251 | | 13 | | 13 | 2 | 12 | 4 | 4 | _ | - |
| Chain | | | ¥ | ٧ | | A | | A | Ą | ¥ | A | A | 4 | 4 |
| eg a | | lcvl | lei9 | lex9 | | lax4 | | 1bj4 | 1cOn | 1cj0 | lcsl | 1dfo | leg5 | leg5 |
| SEQ Sign | | 834 | 834 | 834 | | 836 | | 836 | 836 | 836 | 836 | 836 | 836 | 836 |

| PDB annotation | TRANSFERASE SHMT; SERINE- GLYCINE CONVERSION, PYRIDOXAL 5'-PHOSPHATE, 2 TETRAHYDROFOLATE, ASYMMETRIC DIMER | LYASE FES CLUSTER BIOSYNTHESIS, PYRIDOXAL 5-PHOSPHATE, 2 THIOCYSTEINE, AMINOACRYLATE, ENZYME-PRODUCT COMPLEX | CARBOXYLIC ESTER HYDROLASE PHOSPHOLIPASE, TRIMER, CALCIUM BINDING, ACTIVATOR SITE, 2 CARBOXYLC ESTER HYDROLASE | HYDROLASE PLAZ, PHOSPHATIDE SN-2 ACYLHYDROLASE; HYDROLASE, PHOSPHOLIPASE AZ, LIPID DEGRADATION, PRESYNAPTIC 2 NEUROTOXIN, VENOM | HYDROLASE HYDROLASE, PHOSPHOLIPASE A2, PLATELET AGGREGATION INHIBITOR, 2 PBPB HEADER MODRES | | | | | LIPID DEGRADATION PHOSPHOLIPASE A2, LIPID |
|------------------|--|---|---|---|--|--|---|--|---|--|
| Coumpound | SERINE HYDROXYMETHYLTRANSF ERASE; CHAIN: A, B, C, D; | L-CYSTEINE/L-CYSTINE C-S LYASE; CHAIN: A, B; | PHOSPHOLIPASE A2; CHAIN: NULL; | PHOSPHOLIPASE A2; CHAIN: NULL; | PHOSPHOLIPASE A2; CHAIN: NULL; | HYDROLASE PHOSPHOLIPASE A2 (E.C.3.1.14) IPOA 3 | HYDROLASE PHOSPHOLIPASE A2 (B.C.3.1.1.4) COMPLEX WITH THE IPOC 3 TRANSITION- SITATE ANALOGUE IPOC 4 | HYDROLÁSE PHOSPHOLIPASE A2 (E.C.3.1.1.4) COMPLEX WITH THE IPOC 3 TRANSITION- STATE ANALOGUE IPOC 4 | HYDROLASE CALCIUM- FREE PHOSPHOLIPASE A=2= (E.C.3.1.1.4) IPP2 4 | PHOSPHOLIPASE A2; CHAIN: A, B; |
| SeqFold score | | | | | | | 99.59 | | | |
| PMF | -0.11 | 0.83 | .0.08 | -0.18 | -0.13 | -0.14 | | 0.21 | -0.14 | -0.17 |
| Verify score | 0.41 | -0.03 | 0.38 | 0.07 | 0.07 | 0.3 | | 0.08 | 0.2 | 0.12 |
| PSI- BLAST | 7.20E-35 | 3.90E-28 | 4.80E-39 | 4.80E-41 | 1.60E-40 | 1.60E-38 | 1.40E-36 | 0.0054 | 1.60E-38 | 3.20E-44 |
| End | 246 | 241 | 234 | 244 | 253 | 234 | 289 | 438 | 253 | 253 |
| Start AA | 12 | 1 | 131 | 131 | 131 | 131 | 151 | 355 | . 181 | 131 |
| Chain D | ¥ | ۷ | | | | | | | R | ٧ |
| 80 ea | leji | lelu | 1a3d | lae7 | 1bk9 | 1poa | Ірос | 1 poc | lpp2 | lvap |
| S e S | 836 | 836 | 837 | 837 | 837 | 837 | 837 | 837 | 837 | 837 |

| | _ | | | , | | | | , | | | | |
|------------------|------------------------|--|---|--|-------------------------------|---|---|---|---|---|---|--|
| PDB annotation | DEGRADATION, HYDROLASE | HYDROLASE HYDROLASE, PHOSPHOLIPASE A2, ANTICOAGULANT | HYDROLASE HYDROLASE, LIPID DEGRADATION, CALCIUM, PRESYNAPTIC 2 NEUROTOXIN, VENOM | | | OXIDOREDUCTASE PDZ DOMAIN, NNOS, NITRIC OXIDE SYNTHASE | PEPTIDE RECOGNITION PEPTIDE RECOGNITION, PROTEIN LOCALIZATION | PEPTIDE RECOGNITION PEPTIDE RECOGNITION, PROTEIN LOCALIZATION | CYTOKINE LCF; CYTOKINE, LYMPHOCYTE CHEMOATTRACTANT FACTOR, PDZ DOMAIN | CYTOKINE LCF; CYTOKINE, LYMPHOCYTE CHEMOATTRACTANT PACTOR, PDZ DOMAIN | KINASE HCASK, GLGF REPEAT, DHR; PDZ DOMAIN, NEUREXIN, SYNDECAN, RECEPTOR CLUSTERING, KINASE | SIGNAL TRANSDUCTION HDLG, DHR3 DOMAIN; SIGNAL |
| Coumpound | | PHOSPHOLIPASE A2; CHAIN: NULL; | PHOSPHOLIPASE A2; CHAIN: A, B; | HYDROLASSICABOXYL ESTER) PHOSPHOLIPASE A-2- (PHOSPHATIDE 2- ACYL-HYDROLASE) MUTANT 3P24 WITH ARP SPER-ACED BY SER, SER ORDELACED BY CRI, SER SA-6- SELETTED, ASN 677 REPLACED BY TYR, 3P2 6- (IC)5983, S6065, DELETD, ASN 677 (IC)5983, R6065, DELETD, R6 | /NO/ 13) (E.C.3.1.1.4) 3F2F / | NEURONAL NITRIC OXIDE SYNTHASE; CHAIN: A; HEPTAPEPTIDE; CHAIN: B; | PSD-95; CHAIN: A; CRIPT; CHAIN: B; | PSD-95; CHAIN: A; CRIPT; CHAIN: B; | INTERLEUKIN 16; CHAIN: NULL; | INTERLEUKIN 16, CHAIN: NULL; | HCASK/LIN-2 PROTEIN; CHAIN: A, B; | HUMAN DISCS LARGE PROTEIN; CHAIN: NULL; |
| SeqFold score | | | | | | | | | | | | |
| PMF score | | -0.11 | -0.08 | 90'0- | | 86.0 | 0.72 | 0.1 | 66'0 | 0.45 | 0.66 | 0.88 |
| Verify score | | 0.15 | 0.4 | 0.34 | | 0.79 | 0.21 | -0.25 | 0.59 | -0.03 | 9.04 | 0.45 |
| PSI- BLAST | | 4.80E-41 | 1.30E-40 | 1.60E-38 | | 1.30E-13 | 1.10E-18 | 6.40E-10 | 7.20E-16 | 1.40E-14 | 1.30E-14 | 6.40E-17 |
| End | | 248 | 244 | 236 | | 901 | 102 | 317 | 601 | 801 | 801 | 113 |
| Start | | 131 | 131 | 132 | | 21 | | 254 | 21 | 4 | 21 | 20 |
| Chain | | | ¥ | ∢ | | ¥. | ⋖ | ¥ | | | 4 | |
| 808 OI | | lvip | Znot | 3р2р | | 1Ъ8q | 1be9 | 1be9 | 1116 | 1116 | lkwa | 1 pdr |
| SEQ B B S | | 837 | 837 | 837 | | 838 | 838 | 838 | 838 | 838 | 838 | 838 |

| PDB annotation | TRANSDUCTION, SH3 DOMAIN, REPEAT | OXIDOREDUCTASE BETA-FINGER | MEMBRANE PROTEINOXIDOREDUCTASE BETA- FINGER, HETERODIMER | PEPTIDE RECOGNITION PSD-95; PDZ DOMAIN, NEURONAL NITRIC OXIDE SYNTHASE, NMDA RECEPTOR 2 BINDING | HYDROLASE PDZ DOMAIN, HUMAN PHOSPHATASE, HPTP1E, PTP-BAS, SPECIFICITY 2 OF BINDING | OXIDOREDUCTASE (D, L) STEREOSPECIFIC OPINE DEHYDROGENASE, OXIDOREDUCTASE | OXIDOREDUCTASE OXYDOREDUCTASE | TRANSFERASE TRANSFORMYLASE, PURINE BIOSYNTHESIS, ATP-GRASP | OXIDOREDUCTASE LYSINE BIOSYNTHESIS, ALPHA. AMINOADIPATE PATHWAY, 2 SACCHAROPINE REDUCTASE, DEHYDROGENASE | OXIDOREDUCTASE OXIDOREDUCTASE, OXIDOREDUCTASE, NAD | TRANSFORMING GROWTH FACTOR OSTEOGENIC PROTEIN-1, HOP-1, |
|-----------------|-------------------------------------|---|--|--|--|--|--|---|--|--|---|
| Coumpound | | NEURONAL NITRIC OXIDE SYNTHASE (RESIDUES 1- 130); CHAIN: A; | ALPHA-I SYNTROPHIN (RESIDUES 77-I7); CHAIN: A; NEURONAL NITRIC OXIDE SYNTHASE (RESIDUES 1-130; CHAIN: B; | POSTSYNAPTIC DENSITY PROTEIN 95; CHAIN: A; | TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1); CHAIN: A; | N-(I-D-CARBOXYLETHYL)- L-NORVALINE DEHYDROGENASE; CHAIN: NULL: | GLYCERALDEHYDE-3- PHOSPHATE DEHYDROGENASE; CHAIN: P, R, O, Q; | PHOSPHORIBOSYLGLYCINA MIDE FORMYLTRANSFERASE 2; CHAIN: A, B; | SACCHAROPINE REDUCTASE; CHAIN: A; | L-ALANINE DEHYDROGENASE; CHAIN: A; | BONE MORPHOGENETIC PROTEIN-7; CHAIN: NULL; |
| SeqFold | | | | | | | | • | | | |
| PMF | | 0.57 | 0.86 | _ | 0.45 | 0.17 | 60.0 | 0.05 | - | 0.49 | _ |
| Verify score | | -0.12 | 0.49 | 0.28 | -0.09 | -0.18 | -0.1 | -0.09 | 1.04 | -0.24 | 0.14 |
| PSI- BLAST | | 9.00E-15 | 3.20E-17 | 1.40E-18 | 6.40E-17 | 1.60E-05 | 6900:0 | 0.0054 | 4.80E-58 | 1.30E-61 | 9.60E-48 |
| End AA | | 901 | 103 | 107 | 66 | 594 | 570 | 599 | 924 | 460 | 213 |
| Start AA | | 21 | 20 | 20 | | 481 | 480 | 482 | 481 | 25 | 112 |
| Chain ID | | ∢ | ¥ | ∢ | ٨ | | e. | 4 | v | ٧ | |
| <u> </u> | | Iqau | lqav | ląlc | 3pdz | 1bg6 | 1cf2 | leyz | <u>8</u> | 1pjc | т Б |
| S e S | | 838 | 838 | 838 | 838 | 840 | 840 | 840 | 840 | 840 | 842 |

| PDB annotation | BMP-7; MORPHOGEN, TRANSFORMING GROWTH FACTOR, CYTOKINE, BONE, 2 CARTILAGE, GLYCOPROTEIN | TRANSFORMING GROWTH FACTOR OSTBOGRADC PROTEIN-1, HOP-1, BMP-7; MORPHOGRY, TRANSFORMING GROWTH FACTOR, CYTOKINE, BONE, 2 CARTILAGE, GLYCOROTEIN | | | | CYTOKINE CYTOKINE, BONE MORPHOGENETIC PROTEIN, CYSTIN- KNOT, TGFB- 2 FAMILY | HYDROLASE TETRATRICOPEPTIDE, TRP, HYDROLASE, PHOSPHATASE, PROTEIN-PROTEIN INTERACTIONS, TPR, 2 SUPER-HELIX, X-RAY STRUCTURE | HYDROLASE TETRATRICOPEPTIDE, TRP; HYDROLASE, PHOSPHATASE, PROTEIN-PROTEIN INTERACTIONS, TPR, 2 SUPER-HELIX, X-RAY STRUCTURE | HYDROLASE TETRATRICOPEPTIDE, TRP: HYDROLASE, PHOSHATASE, PROTEIN-PROTEIN INTERACTIONS, TPR, 2 SUPER-HELLX, X-RAY STRUCTURE |
|-----------------|--|--|---|---|--|---|---|---|--|
| Coumpound | | BONE MORPHOGENETIC PROTEIN-7; CHAIN: NULL; | GROWTH FACTOR TRANSFORMING GROWTH FACTOR-BETA TWO (TGF- B2) 2TGI 3 | GROWTH FACTOR TRANSFORMING GROWTH FACTOR-BETA TWO (TGF- B2) 2TGI 3 | GROWTH FACTOR TRANSFORMING GROWTH FACTOR-BETA TWO (TGF- B2) 2TGI 3 | BONE MORPHOGENETIC PROTEIN 2 (BMP-2); CHAIN: A; | SERINE/THREONINE PROTEIN PHOSPHATASE 5; CHAIN: NULL; | SERINE/THREONINE PROTEIN PHOSPHATASE 5; CHAIN: NULL; | SERINETHREONINE PROTEIN PHOSPHATASE 5; CHAIN: NULL; |
| SeqFold | | 104.28 | 67.81 | | | | | | |
| PMF score | | | | 0.81 | 0.6 | _ | 0.25 | 0.11 | 8.0 |
| Verify score | | | | 0.04 | 0.11 | 0.05 | 0.16 | 0.23 | 0.47 |
| PSI- BLAST | | 9.60E-48 | 1.80E-38 | 1.60E-36 | 1.80E-38 | 4.80E-48 | 0.00013 | 1.60E-07 | 1.40E-05 |
| End AA | | 214 | 214 | 213 | 213 | 213 | 909 | 805 | 1103 |
| Start AA | | 112 | 100 | 102 | 112 | Ξ. | 430 | 999 | 392 |
| Chain ID | | * | | | | ٧ | | | |
| PDB ID | | 1bm p | 2tgi | 2tgi | 2tgi | 3bm p | la17 | lal7 | la17 |
| SEQ NO: | | 842 | 842 | 845 | 842 | 842 | 843 | 843 | 843 |

| PDB annotation | KINASE KINASE, SH3 DOMAIN, TRANSFEBASE, PHOSPHOTRANSFERASE, 2 PROTO- ONCOGENE, MULTIPLE DOMAIN, LEUKEMA | COMPLEX (SHE DOWAINVIRAL BINHANCER) SRC-HOMOLOGY 3 DOMANY/WALA ERHANCER), RPOTO- ONCOGENE, 2 TRANSPERASE, TYROSINE-PROTEIN KINASE, HOSPHORYLATION, 3 AIDS. AFF-BINDING, STB DOMAIN, 8TH2 DOMAN, PPII HELJS, PXXP MOTTE. | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELICAL REPEAT, HSP90, 2 PROTEIN BINDING | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELICAL REPEAT. HSP90, 2 PROTEIN BINDING | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELICAL REPEAT, HSP90, 2 PROTEIN BINDING | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELICAL REPEAT, HSP90, 2 PROTEIN BINDING | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELLCAL REPEAT, HSC70, 2 HSP70, PROTEIN BINDING | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELJCAL REPEAT, HSC70, 2 HSP70, PROTEIN BINDING | CHAPERONE HOP, TPR-DOMAIN, PEPTIDE-COMPLEX, HELJCAL REPEAT, HSC70, 2 HSP70, PROTEIN BINDING | SIGNALING PROTEIN PEROXISMORE RECEPTOR 1, PTSI-BP, PEROXIN-5, |
|------------------|---|---|--|--|--|--|--|---|---|---|
| Coumpound | ABL TYROSINE KINASE; CHAIN: NULL; | FYN TROSINE KINASE; CHAIN: A.C, HIV.1 NEF PROTEIN, CHAIN: B, D, | TPR2A-DOMAIN OF HOP; CHAIN: A; HSP90-PEPTIDE MEEVD; CHAIN: B; | TPR2A-DOMAIN OF HOP; CHAIN: A; HSP90-PEPTIDE MEEVD; CHAIN: B; | TPRZA-DOMAIN OF HOP: CHAIN: A; HSP90-PEPTIDE MEEVD; CHAIN: B; | TPR2A-DOMAIN OF HOP; CHAIN: A; HSP90-PEPTIDE MEEVD; CHAIN: B; | TPR1-DOMAIN OF HOP; CHAIN: A, B; HSC70- PEPTIDE; CHAIN: C, D; | TPR1-DOMAIN OF HOP; CHAIN: A, B; HSC70- PEPTIDE; CHAIN: C, D; | TPR1-DOMAIN OF HOP; CHAIN: A, B; HSC70- PEPTIDE; CHAIN: C, D; | PEROXISOMAL TARGETING SIGNAL I RECEPTOR; |
| SeqFold score | | | | | | | | | | |
| PMF | 99.0 | 0.19 | 0.57 | 90'0 | 0.04 | 0.22 | 80.0- | 60:0 | 90:0 | 0.75 |
| Verify | 0.22 | 0.46 | 0.32 | 0.11 | -0.02 | 90.0- | 0.02 | 0.24 | 0.33 | 0.22 |
| PSI- BLAST | 1.30E-06 | 7.20E-08 | 1.10E-05 | 9.60E-08 | 8.00E-08 | 3.20E-10 | 6.40E-11 | 0.00014 | 1.10E-06 | 9.00E-07 |
| End | 242 | 242 | 594 | 526 | 815 | 888 | 1119 | 575 | 873 | 109 |
| Start AA | 193 | | 432 | 452 | 720 | 783 | 0001 | 441 | 742 | 375 |
| Chain ED | | ∢ | ¥ | ¥ | ¥ | . V | ¥ | ¥ | ¥ | ¥ |
| E CE | lawo | lefin. | 1elr | lelr | 1clr | lelr | lclw | Iclw | lelw | 1fch |
| SEQ B B SE | 843 | 843 | 843 | 843 | 843 | 843 | 843 | 843 | 843 | 843 |

| | | | | | | | | _ |
|-----------------|---|---|--|---|--|---|---|-------------------------------|
| PDB annotation | PTSI PROTEIN-PEPTIDE COMPLEX, TETRATRICOPEPTIDE REPEAT, TPR, 2 HELICAL REPEAT | SIGNALING PROTEIN PEROXISMORE RECEPTOR I, PTSI-BP, PEROXIN-5, PTSI PROTEIN-PEPTIDE COMPLEX, THE RATRICOPPETIDE REPEAT, TPR, 2 THE TOAT PEROFES. | SIGNALING PROTEIN PEROXISMORE RECEPTOR I, PTSI-BP, PEROXIN-5, PTSI PROTEIN-PEPTIDE COMPLEX, TETRATRICOPPTIDE REPEAT, TPR, 2 HELICAL REPEAT | SIGNALING PROTEIN PEROXISMORE RECEPTOR I, PTSI-BP, PEROXIN-5, PTSI PROTEIN-PEPTIDE COMPLEX, TETRATRICOPEPTIDE REPEAT, TPR, 2 HEJICAL REPEAT | TRANSFERASE PROTO-ON/COGENE TYROSINE KINASE, PROTO- ONCOGENE, TRANSFERASE, TYROSINE-PROTEIN KINASE, 2 PHOSPHORYLATION, ATP-BINDING, MYRISTYLATION, SH3 DOMAIN, 3 COMPLEX COMPLEX | | COMPLEX (KINASEPEPTIDE) | COMPLEX (TRANSFERASE/PEPTIDE) |
| Coumpound | CHAIN: A, B; PTSI. CONTAINING PEPTIDE; CHAIN: C, D; | PEROXISOMAL TARGETING SIGNAL I RECEPTOR; CHAIN: A, B; PTSI- CONTAINING PEPTIDE; | PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR; CHAIN: A, B; PTS1- CONTAINING PEPTIDE; CHAIN: C, D. | PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR; CHAIN: A, B; PTSI- CONTAINING PEPTIDE; CHAIN: C, D; | PHOSPHOTRANSFERASE FYN, CHAIN: A; 3BP-2; CHAIN: B; | PROTEIN GROWTH FACTOR RECEPTOR-BOUND FROTEN 3 STA DOMAN COMPLEXED WITH SOS-A PETIDE IGRA 4 (NMR, 29 STRUCTURES) IGRS, STRUCTURES) IGRS, | P56=LCK = TYROSINE KINASE; ILCK 7 CHAIN: A; ILCK 8 TAIL PHOSPHOPETIDE TEGQPHOSPHO)YQPQPA; ILCK 14 CHAIN: B: ILCK 15 | C-SRC; CHAIN: C; NL1 (MN7- |
| SeqFold | | | | | | | | |
| PMF score | | 0.62 | -0.15 | 0.99 | 9.4 | 0.59 | 0.28 | 0.29 |
| Verify score | | 0.29 | 90:0 | 0.02 | 0.23 | 0.74 | 60.0 | 4.0 |
| PSI- BLAST | | 3.60E-09 | 1.30E-20 | 1.10E-12 | I.80E-07 | 1,40E-06 | 1.80E-05 | 1.80E-07 |
| End AA | | 804 | 669 | 842 | 242 | 249 | 288 | 242 |
| Start AA | | 445 | 452 | 576 | 193 | 181 | 193 | 193 |
| Chain ID | | ¥ | Ą | ¥ | ¥ | | ¥ | C |
| PDB ID | | 1fch | Ifch | fg. | 1fyn | 1gbr | 11ck | ln6 |
| SEQ No: d | | 843 | 843 | 843 | 843 | 843 | 843 | 83 |

| PDB annotation | SRC, SH3 DOMAIN, LIGANDS, NON- PEPTIDE ELEMENTS, 2 COMPLEX (TRANSFERASE/PEPTIDE) | | TYROSINE KINASE TYROSINE KINASE-INHIBITOR COMPLEX, DOWN-REGULATED KINASE, 2 ORDERED ACTIVATION LOOP | PROTEIN TRANSPORT HELIX-TURN- HELIX TPR-LIKE REPEAT, PROTEIN TRANSPORT | PROTEIN TRANSPORT HELIX-TURN- HELIX TPR-LIKE REPEAT, PROTEIN TRANSPORT | | TRANSFERASE HCK; SH3, PROTEIN TYROSINE KINASE, SIGNAL TRANSDUCTION, 2 TRANSFERASE | IMMUNOGLOBULIN | IMMUNOGLOBULIN IMMUNOGLOBULIN, FAB FRAGMENT, HUMANISATION | COMPLEX (VIRAL CASEDIMANINOGLOBULIN) HIV-1 CA, HIV DA, HIV PA, P24; FAB LIGHT CHAIN, FAB HEAVY CHAIN COMPLEX (VIRAL CAPSID/MANINOGLOBULIN), HIV, |
|-----------------|--|---|--|--|--|--|---|--|---|--|
| Coumpound | MN2-MN1-PLPPLP); CHAIN: N; | PHOSPHOTRANSFERASE PHOSPHATUROSTROL 3- KINASE (P85-ALPHA SUBUNT, IPNI 3 SH3 DOMALIN (NMR, MINIMIZED AVERAGE STRUCTURE) IPNI 4 | HAEMATOPOETIC CELL KINASE (HCK), CHAIN: A; | VESICULAR TRANSPORT PROTEIN SEC17; CHAIN: A; | VESICULAR TRANSPORT PROTEIN SEC17; CHAIN: A; | PHOSPHOTRANSFERASE FYN PROTO-ONCOGENE TYROSINE KINASE (E.C.2.7.1.112) 1SHF 3 (SH3 DOMAIN) 1SHF 4 | HEMATOPOIETIC CELL KINASE; CHAIN: NULL; | 2E8 (IGGI=KAPPA=) ANTIBODY; CHAIN: L, H, M, P; | ANTIBODY CTM01; CHAIN: L, H; | HUMAN IMMUNODEFICIENCY VIRUS TYPE I CAPSID CHAIN: A. B; ANTIBODY FAB25.3 ANTIBODY FAB26.3 M: |
| SeqFold | | | | | | | | | | |
| PMF | | 0.17 | 0.17 | 0.15 | 60.0 | 0.54 | 0.89 | -0.06 | 0.03 | 0.24 |
| Verify score | | 0.54 | 60:0 | 0.06 | -0.03 | 0.38 | 0.45 | 80.0 | -0.18 | 0.05 |
| PSI- BLAST | | 9.00E-10 | 3.60E-07 | 1.80E-07 | 8.00E-06 | 9.00E-08 | 9.00E-06 | 6.40E-51 | 4.80E-53 | 4.80E-63 |
| End AA | | 249 | 282 | 573 | 1011 | 242 | 255 | 414 | 299 | 220 |
| Start AA | | 182 | 163 | 418 | 949 | | 193 | 236 | 419 | 21 |
| Chain | | , | 4 | ٧ | ¥ | ∢ | | н | н | Н |
| PDB U | | Ē | ldcf | lqqe | 1qqe | Ishf | 4hck | 1.20 E+09 | lac6 | lafv |
| SEQ NO DE | | 843 | 843 | 843 | 843 | 843 | 843 | 846 | 846 | 846 |

| PDB annotation | CAPSID PROTEIN, 2 P24 | INSECT IMMUNITY INSECT IMMUNITY, LPS-BINDING, HOMOPHILIC ADHESION | INSECT IMMUNITY INSECT | IMMUNITY, LPS-BINDING, HOMOPHILIC ADHESION | INSECT IMMUNITY INSECT IMMUNITY, LPS-BINDING. | HOMOPHILIC ADHESION | INSECT IMMUNITY INSECT IMMUNITY, LPS-BINDING, HOMOPHILC ADHESION | INSECT IMMUNITY INSECT IMMUNITY, LPS-BINDING, HOMOPHILIC ADHESION | RECEPTOR RECEPTOR, SIGNAL | TRANSDUCER OF IL-6 TYPE | CYTOKINES, THIRD 2 N-TERMINAL DOMAIN, TRANSMEMBRANE. | GLYCOPROTEIN | IMMUNE SYSTEM | IMMUNOGLOBULIN, IMMUNE | SYSTEM | | IMMUNOGLOBULIN | IDIOTOPE, ANTI-IDIOTOPE | | | | IMMUNE SYSTEM | IMMUNOGLOBULIN, IGG1; | IMMINOGLOBULIN, IGGI FAB | FRAGMENT, CROSS-REACTIVITY | HIV1 PROTEASE, ENZYME 2 | IMMUNE SYSTEM ANTI-PRION FAB |
|------------------|-----------------------|---|------------------------|---|---|---------------------|--|---|---------------------------|-------------------------|--|--------------|---------------------|------------------------|--|----------------------|------------------|-------------------------|--------------------------|-------------------------|-------------------------------------|--------------------|--------------------------|--------------------------|----------------------------|-------------------------|------------------------------|
| Coumpound | | HEMOLIN; CHAIN: A, B; | HEMOLIN; CHAIN: A, B; | | HEMOLIN; CHAIN: A, B; | | HEMOLIN; CHAIN: A, B; | HEMOLIN; CHAIN: A, B; | GP130; CHAIN: NULL; | | | | MONOCLONAL ANTIBODY | MRK-16 (LIGHT CHAIN); | CHAIN: A, C; MONOCLONAL ANTIBODY MRK-16 (HEAVY | CHAIN); CHAIN: B, D; | IG HEAVY CHAIN V | HEAVY CHAIN V REGIONS: | CHAIN: B; IG HEAVY CHAIN | V REGIONS; CHAIN: C; IG | HEAVY CHAIN V REGIONS; CHAIN: D: | IGGI ANTIBODY 1696 | (LIGHT CHAIN); CHAIN: L; | (VARIARI F HEAVY CHAIN): | CHAIN: H: IGGI ANTIBODY | 1696 (CONSTANT HEAVY | FAB ANTIBODY LIGHT |
| SeqFold score | | 159.92 | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | | _ | | 0.54 | | 99:0 | 0.21 | -0.05 | | | | 0.04 | | | | -0.13 | | | | | -0.19 | | | | | -0.11 |
| Verify score | | | 0.28 | | 0.29 | | 0.15 | 0.14 | 0.07 | | | | 96.0 | | | | 0.17 | | | | | 0.03 | | | | | 90:0 |
| PSI- BLAST | | 5.40E-62 | 5.40E-62 | | 1.60E-31 | | 7.20E-48 | 3.20E-22 | 1.40E-12 | | | | 3.20E-64 | | | | 1.60E-49 | | | | | 6.40E-23 | | | | | 3.20E-49 |
| End | | 503 | 503 | | 493 | | 404 | 713 | 265 | | | | 220 | | | | 412 | | | | | 603 | | | | | 415 |
| Start | | 134 | 135 | | 138 | | 27 | 323 | 208 | | | | 21 | | | | 235 | | | | | 523 | | | | | 236 |
| Chain ID | | ¥ | Ą | | V | | ¥ | ¥ | | | | | В | | | | œ | | | | | _ | | | | | н |
| PDB ID | | 녎 | 1bih | | ųq 1 | | 16ih | Hall Hall | 1bj8 | | | | Ibln | | | | je je | | | | | lcl7 | | | | | lcr9 |
| SEQ NO: | | 846 | 846 | | 846 | | 846 | 846 | 846 | | | | 846 | | | | 846 | | | | | 846 | | | | | 846 |

| | | | | | | | | | | _ | | | | | _ | | | | | | _ | | | | | | |
|------------------|---|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|-----------------------------|------------------------|-----------------------------|-------------------------------|--------------------------------------|-----------------------------|------------------------|-------------------------------|-----------------------------|----------|-----------------------------|------------------------|-----------------------------|-----------------------------|----------|-----------------------------|------------------------|---|
| PDB annotation | 3F4; ANTI-PRION FAB 3F4 ANTI-PRION ANTIBODY, FAB 3F4 | CELL ADHESION NEURAL CELL ADHESION | CELL ADHESION NEURAL CELL ADHESION | CELL ADHESION NEURAL CELL ADHESION | CELL ADHESION NEURAL CELL ADHESION | CELL ADHESION NEURAL CELL ADHESION | CELL ADHESION NEURAL CELL ADHESION | CELL ADHESION NEURAL CELL ADHESION | CELL ADHESION NEURAL CELL ADHESION | GROWTH FACTOR/GROWTH FACTOR | RECEPTOR FGF, FGFR, | IMMUNOGLOBULIN-LIKE, SIGNAL | CROWNER BACTOR/CROWNER EACTOR | GROWIN FACTOR GROWTH FACTOR RECEPTOR | GROWTH FACTOR/GROWTH FACTOR | RECEPTOR FOF, FOFR, | TRANSDICTION, 2 DIMERIZATION. | GROWTH FACTOR/GROWTH FACTOR | RECEPTOR | GROWTH FACTOR/GROWTH FACTOR | RECEPTOR FGF, FGFR, | IMMUNOGLOBULIN-LIKE, SIGNAL | GROWTH FACTOR/GROWTH FACTOR | RECEPTOR | GROWTH FACTOR/GROWTH FACTOR | RECEPTOR FGF, FGFR, | IMMUNOCLOBOLIN-LINE, SIGNAL TRANSDUCTION, 2 DIMERIZATION, |
| Coumpound | CHAIN; CHAIN: I.; FAB ANTIBODY HEAVY CHAIN; CHAIN: H; | AXONIN-1; CHAIN: A; | AXONIN-1; CHAIN: A; | AXONIN-1; CHAIN: A; | AXONIN-1; CHAIN: A; | AXONIN-1; CHAIN: A; | AXONIN-1; CHAIN: A; | AXONIN-1; CHAIN: A; | AXONIN-1; CHAIN: A; | FIBROBLAST GROWTH | FACTOR 2; CHAIN: A, B; | FIBROBLAST GROWTH | FACTOR RECEPTOR 1; | CHAIN: C, D, | FIBROBLAST GROWTH | FACTOR 2; CHAIN: A, B; | FACTOR RECEPTOR 1: | CHAIN: C, D; | | FIBROBLAST GROWTH | FACTOR 2; CHAIN: A, B; | FIBROBLASI GROWIN | CHAIN: C. D. | | FIBROBLAST GROWTH | FACTOR 2; CHAIN: A, B; | FIGUREASI ORUWIN |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | _ | _ | 0.43 | -0.14 | 96'0 | - | 0.58 | 0.51 | 0.94 | | | | | 0.22 | | | | | 0.99 | | | | | -0.03 | | |
| Verify score | | 80.0 | 0.24 | -0.14 | 0.02 | 0.23 | 0.13 | 0.07 | 0.07 | 0.15 | | | | | 0.07 | | | | | 0.22 | | | | | 0.26 | | |
| PSI- BLAST | | 3.60E-59 | 4.80E-45 | 1.60E-47 | 1.10E-37 | 1.80E-44 | 6.40E-42 | 1.60E-53 | 3.20E-33 | 1.80E-30 | | | | | 3.20E-21 | | | | | 1.80E-32 | | | | | 8.00E-21 | | |
| End | | 503 | 203 | 321 | 412 | 265 | 709 | 4 4 4 4 | 713 | 320 | | | | | 109 | | | | | 320 | | | | | 109 | | |
| Start | | 135 . | 138 | 2 | 20 | 226 | 236 | 24 | 320 | 135 | | | | | 430 | | | | | 135 | | | | | 430 | | |
| Chain | | ¥ | ¥ | ¥ | ¥ | ٧ | ٧ | ∢ | ¥ | ပ | | | | | ၁ | | | | | Ω | | | | | Ω | | |
| 908 ED (E) | | lcs6 | 1cs6 | 1036 | 1036 | lcs6 | 9501 | 1cs6 | 1cs6 | lcvs | | | | | Icvs | | | | | lcvs | | | | | lcvs | | |
| SEQ B B SE | | 846 | 846 | 846 | 846 | 846 | 846 | 846 | 846 | 846 | | | | | 846 | | | | | 846 | | | | | 846 | | |

| | | | | | | | | | | - |
|-----------------|---|--|--|--|--|---|--|--|---|---|
| PDB annotation | GROWTH FACTOR/GROWTH FACTOR RECEPTOR | VIRUS/VIRAL PROTEIN, RECEPTOR CD155, PVR, HUMAN POLIOVIRUS, ELECTRON MICROSOPY, 2 POLIOVIRUS-RECEPTOR COMPLEX, VIDITS/VIDA 1 PROFIEM PECTEN POLIOVIRUA 1 PROFIEM PECTEN PROFISOR PROFIS | VIRLOS TRADELIN RECEPTOR CD155, PVR, HUMAN POLIOVIRUS, ELECTRON MICROSCOPY, 2 POLIOVIRUS-RECEPTOR VIRLINVIRA I PROTEIN PROFEN. | VIRUSVIRAL PROTEIN, RECEPTOR CD155, PVR, HUMAN POLIOVIRUS, ELECTRON MICROSCOPY, 2 POLIOVIRUS-RECEPTOR COMPLEX, VIRUSVIRAL PROTEIN PROFEN PRO | IMMUNE SYSTEM FC IGG PHAGE DISPLAY PEPTIDE | IMMUNE SYSTEM IMMUNOGLOBULIN FOLD, ANTIBODY, IGM, FV | COMPLEX (ANTIBODY ANTIGEN) 1,4— BETA-N-ACETTAMIRABISE C; SINGLE-DOMAIN ANTIBODY, TURKEY EGG-WHITE LYSOZYME, 2 ANTIBODY-PROTEIN COMPLEX, SINGLE-CHAN PY PRAGMEN; | CELL ADHESION NCAM; NCAM, IMMUNGLOBULN FOLD, GLYCOPROTEN | CELL ADHESION NCAM; IMMUNOGLOBULIN FOLD, GLYCOPROTEIN | GROWTH FACTOR/GROWTH FACTOR RECEPTOR FGF2; FGFR2; IMMUNOGLOBULIN (IG)LIKE |
| Coumpound | CHAIN: C, D; | POLIOVIRUS RECEPTOR; CHAIN: R; VP1; CHAIN: 1; VP2; CHAIN: 2; VP3; CHAIN: 3; VP4; CHAIN: 4; | POLIOVIRUS RECEPTOR; CHAIN: R; VP1; CHAIN: 1; VP2; CHAIN: 2; VP3; CHAIN: 3; VP4; CHAIN: 4; | POLIOVIRUS RECEPTOR; CHAIN: R; VP1; CHAIN: 1; VP2; CHAIN: 2; VP3; CHAIN: 3; VP4; CHAIN: 4; | IMMUNOGLOBULIN LAMBDA HEAVY CHAN; CHAIN: A, B; ENGINEERED PEPTIDE: CHAIN: E. F. | IGM MEZ IMMUNOGLOBULN; CHAIN: L; IGM MEZ IMMUNOGLOBULN; CHAIN: H: | SČEV FRAGMENT 1F9; CHAIN: A, B; TURKEY BGG- WHITE LYSOZYME C; CHAIN: X, Y; | NEURAL CELL ADHESION MOLECULE; CHAIN: A, B, C, D: | NEURAL CELL ADHESION MOLECULE; CHAIN: A, B, C, D; | FIBROBLAST GROWTH FACTOR 2; CHAIN: A, B, C, D; FIBROBLAST GROWTH |
| SeqFold | | | | | | | | | | |
| PMF score | | 0.65 | 0.21 | 10.0 | 0.05 | 90.0 | -0.03 | 6.0 | 0.78 | 96:0 |
| Verify score | | -0.3 | -0.31 | 4.0 | -0.27 | 0.00 | 0.14 | 0.34 | 0.37 | 0.07 |
| PSI- BLAST | | 7.20E-36 | 1.10E-38 | 3.60E-44 | 8.00E-40 | 3.20E-38 | 6.40E-42 | 1.80E-31 | 1.30E-24 | 1.40E-34 |
| End | | 404 | 503 | 319 | 114 | 130 | 506 | 319 | 503 | 320 |
| Start | | 141 | 228 | 28 | 234 | 21 | 21 | 142 | 324 | 135 |
| Chain ID | | x | ~ | æ | ¥ | н | ¥ | ¥ | Y | 3 |
| PDB CI | | ldgi | 1dgi | Idgi | Idn2 | 144 | qzp1 | lepf | lepf | lev2 |
| S e S | | 846 | 846 | 846 | 846 | 846 | 846 | 846 | 846 | 846 |

| | | | | | _ | | | | _ | | | | _ | | _ | _ | | _ | | | | | _ | | _ | _ | | _ | | |
|------------------|--|---|-------------------------|---------------------------|-----------------------------|------------------------------|---|---------------------------|--|------------------------------|------------------------------|--------------------------------|---------------------------|-------------------------|-----------------------------|------------------------------|-------------------------|--------------------------------|--|-----------------------------|------------------------|--------------------------|--------------------------------|---------------------------|-----------------------------|------------------------|--------------------------|--------------------------------|---|---|
| PDB annotation | DOMAINS BELONGING TO THE I-SET 2 SUBGROUP WITHIN IG-LIKE DOMAINS, B-TREFOIL FOLD | GROWTH FACTOR/GROWTH FACTOR RECEPTOR FGF2; FGFR2; | IMMUNOGLOBULIN (IG)LIKE | 2 SUBGROUP WITHIN IG-LIKE | GROWTH FACTOR/GROWTH FACTOR | RECEPTOR FGF2; FGFR2; | DOMAINS BELONGING TO THE LSET | 2 SUBGROUP WITHIN IG-LIKE | DOMAINS, B-I REFUIL FULL | GROWTH FACTOR/GROW IN FACTOR | KECEPTOR FORZ; FORKZ; | DOMAINS RELONGING TO THE LISET | 2 SUBGROUP WITHIN IG-LIKE | DOMAINS, B-TREFOIL FOLD | GROWTH FACTOR/GROWTH FACTOR | RECEPTOR FGF2; FGFR2; | IMMUNOGLOBULIN (IG)LIKE | DOMAINS BELONGING TO THE 1-SET | 2 SUBGROUP WITHIN IG-LIKE DOMAINS, B-TREFOIL FOLD | GROWTH FACTOR/GROWTH FACTOR | RECEPTOR FGF1; FGFR1; | IMMUNOGLOBULIN (IG) LIKE | DOMAINS BELONGING TO THE I-SET | 2 SUBGROUP WITHIN IG-LIKE | GROWTH FACTOR/GROWTH FACTOR | RECEPTOR FGF1; FGFR1; | IMMUNOGLOBULIN (1G) LIKE | DOMAINS BELONGING TO THE I-SET | 2 SUBGROUP WITHIN IG-LIKE DOMAINS, B-TREFOIL FOLD | IMMUNE SYSTEM FC-EPSILON RI- ALPHA; IMMUNOGLOBULIN FOLD. |
| Coumpound | FACTOR RECEPTOR 2; CHAIN: E, F, G, H; | FIBROBLAST GROWTH FACTOR 2; CHAIN: A, B, C, D; | FIBROBLAST GROWTH | CHAIN: E, F, G, H; | FIBROBLAST GROWTH | FACTOR 2; CHAIN: A, B, C, D; | FIBRUBLASI GROWIN FACTOR RECEPTOR 2: | CHAIN: E, F, G, H; | THE PART OF THE PARTY OF THE PA | FIBROBLAST GROWTH | FACTOR 2; CHAIN: A, B, C, D; | FACTOR RECEPTOR 2: | CHAIN: E. F. G. H; | | FIBROBLAST GROWTH | FACTOR 2; CHAIN: A, B, C, D; | FIBROBLAST GROWTH | FACTOR RECEPTOR 2; | CHAIN: E, F, G, H; | FIBROBLAST GROWTH | FACTOR 1; CHAIN: A, B; | FIBROBLAST GROWTH | FACTOR RECEPTOR 1; | CHAIN: C, D; | FIBROBLAST GROWTH | FACTOR 1; CHAIN: A, B; | FIBROBLAST GROWTH | FACTOR RECEPTOR 1; | CHAIN: C. D; | HIGH AFFINITY IMMUNOGLOBULIN |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.17 | | | 0.94 | | | | 100 | \$ | | | | - | 0.07 | | | | | 69.0 | | | | | 0.07 | | | | | 0.29 |
| Verify score | | 0.15 | | | 0.23 | | | | 100 | 0.27 | | | | | 0.15 | | | | | 0.11 | _ | | • | | -0.07 | | | | | 0.09 |
| PSI- BLAST | | 7.20E-23 | | | 5.40E-33 | | | | 20000 | 3.60E-24 | | | | | 1.60E-19 | | | | | 1.30E-30 | | | | | 6.40E-20 | | | | | 7.20E-28 |
| End | | 224 | | | 322 | | | | 202 | Š | | | | | 109 | | | | | 320 | | | | | 109 | | | | | 322 |
| Start AA | | 33 | | | 135 | | | | 200 | 579 | | | | | 430 | | | | | 135 | | | | | 430 | | | | | 136 |
| Chain ID | | ш | | | Ü | | Ÿ | | | 5 | | | | | g | | | | | ပ | | | | | U | | | | | 4 |
| 80g E0 | | lev2 | | | lev2 | | | | 2 | Tev2 | | | | | lev2 | | | | | levt | | | | | levt | | | | | 1224 |
| ğ a ÿ | | 846 | | | 846 | | | | 3 | 840 | | _ | | | 846 | | | | | 846 | _ | | | | 846 | | | | | 846 |

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|------------------|---|---|--|---|---|---|--|--|--|---|--|
| PDB annotation | GLYCOPROTEIN, RECEPTOR, IGE- BINDING 2 PROTEIN | IMMUNE SYSTEM ANTI: CARBOHYDRATE ANTIBODY | IMMUNE SYSTEM HIGH APFINITY IGE-FC RECEPTON, FCGESLLON) IGE- FC, IMMUNGGLOBULIN FOLD, GLYCOPROTEIN, RECEPTOR, IGE- BINDING 2 PROTEIN, IGE ANTIBODY, IGE-FC | HÖRMÖNEJGROWTH FACTORHORNONE RECEPTOR 4 FELICAL BUNDLE, ALPHA HELICAL BUNDLE, TERNARY COMPLEX, FN 2 BUNDLE, SEPRET DOMANNS, CYTOKINE-RECEPTOR COMPLEX | | IMMUNE SYSTEM, MEMBRANE PROTEIN CD32; PC RECEPTOR, IMMUNOGLOULIN, LEUKOCYTE, CD32 | HEPARIN AND INTEGRIN BINDING HEPARIN AND INTEGRIN BINDING | IMMUNE SYSTEM RECEPTOR BETA SANDWICH, IMMUNOGLOBULIN- LIKE, RECEPTOR | | | IMMUNOGLOBULIN INTACT IMMUNOGLOBULIN V REGION C |
| Coumpound | EPSILON RECEPTOR CHAIN: A; | ANTBODY S-20-4, FAB FRACMENT, LIGHT CHAIN; CHAIN: L. ANTIBODY S-20-4, FAB FRAGMENT, HEAVY CHAIN: CHAIN: H | HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR CHAIN: A; IG EPSILON CHAIN C REGION; CHAIN B, D; | PLACENTAL LACTOGEN; CHAIN: A; PROLACTIN RECEPTOR; CHAIN: B, C; | IMMUNOGLOBULIN IMMUNOGLOBULIN FC AND FRAGMENT B OF PROTEIN A COMPLEX 1FC2 4 | FC RECEPTOR FC(GAMMA)RIIA; CHAIN: A; | FIBRONECTIN; CHAIN: A; | LOW AFFINITY IMMUNOGLOBULIN GAMMA FC REGION CHAIN: A; | TLYMPHOCYTE ADHESION GLYCOPROTEIN CD2 (HUMAN) IHNF 3 | T LYMPHOCYTE ADHESION GLYCOPROTEIN CD2 (RAT) IHNG 3 | IGG2A INTACT ANTIBODY - MAB231; CHAIN: A, B, C, D |
| SeqFold score | | | | | | | | | | | |
| PMF | | 0 | 0.18 | 0.03 | 0.07 | 0.23 | 0.52 | 0.36 | 9.04 | 0.05 | 0.11 |
| Verify | | 0.02 | 0.17 | 0.05 | -0.03 | -0.16 | 0.17 | -0.02 | -0.31 | 0.03 | -0.16 |
| PSF- BLAST | | 1.60E-62 | 1.10E-29 | 9.00E-15 | 1.10E-39 | 1.10E-24 | 3.60E-17 | 1.80E-22 | 1.60E-21 | 3.60E-27 | 0 |
| End | | 220 | 322 | 715 | 411 | 319 | 708 | 319 | 305 | 319 | 412 |
| Start AA | | 21 | 132 | 524 | 234 | 143 | 512 | 139 | 141 | 143 | 21 |
| Chain | | н | ∢ | Ф | Q | 4 | ٧ | ∢ | | Y | м |
| PDB ID | | Iftw | 1f6a | 116f | 162 | lfcg | 1fth | Ā | lhnf | 1hng | ligt |
| SEQ No: | | 846 | 846 | 846 | 846 | 846 | 846 | 846 | 846 | 846 | 846 |

| PDB annotation | REGION, IMMUNOGLOBULIN | IMMUNOGLOBULIN INTACT IMMUNOGLOBULIN, V REGION, C REGION, HINGE REGION | IMMUNOGLOBULIN INTACT IMMUNOGLOBULIN, V REGION, C REGION, HINGE REGION | COMPLEX: (IMMUNOGLOBULINRECEPTOR) INMUNOGLOBULIN FOLD, TRANSMEMBRANE, GLYCOPROTEIN, RECEPTOR, S JGIGNAL, COMPLEX (IMMUNOGLOBULINRECEPTOR) | COMPLEX (IMMUNOCLOBULINRECEPTOR) TCR (IMMUNOCLOBULINRECEPTOR) TCR VAPILAY VBETA DOMAIN; T-CELL RECEPTOR, STRAND SWITCH, FAB, ANTICCHONTYPIC, C (IMMUNOCLOBULINRECEPTOR) | | | | | |
|-----------------|------------------------|--|--|--|---|--|--|--|---|---|
| Coumpound | | IGGI INTACT ANTIBODY MAB61.1.3; CHAIN: A, B, C, D | IGGI INTACT ANTIBODY MAB61.1.3; CHAIN: A, B, C, D | INTERLEUKIN-I BETA; CHAIN: A; TYPE I INTERLEUKIN-I RECEPTOR; CHAIN: B; | KB5-C20 T-CELL ANTIGEN RECEPTOR; CHAIN: A, B; ANTIBODY DESIRE-1; CHAIN: L, H; | MANUNOGLOBULIN ANTI- HAPSHALINGYLINOSTROL SPECIFIC PHOSPHOLIPASE C DLABODY 11MK 3 SYNONYMS: LSMK16 DLABODY, SINGLE-CHAIN FY DIMER ILMK 4 | IMMUNOGLOBULIN ANTIGEN-BINDING FRAGMENT (FAB) (IGG2B, KAPPA) IMAM 3 | IMMUNOGLOBULIN IMMUNOGLOBULIN GI (IGG1) (MCG) WITH A HINGE DELETION IMCO 3 | IMMUNOCLOBULN IMMUNOCLOBULN GI (IGG1) (MCG) WITH A HINGE DELETION IMCO 3 | IMMUNOGLOBULIN IMMUNOGLOBULIN FAB FRAGMENT (MC/PC\$603) |
| SeqFold | | 110.16 | | | | | | | 123.28 | |
| PMF | | | 0.24 | 0.49 | -0.17 | 0.01 | 0.22 | 0.04 | | 90:0 |
| Verify score | | | -0.05 | 0.21 | 0.11 | -0.23 | -0.05 | -0.17 | | -0.26 |
| PSI- BLAST | | 3.20E-95 | 3.20E-95 | 5.40E-29 | 1.10E-49 | 3.20E-39 | 4.80E-62 | 1.60E-93 | 1.60E-93 | 8.00E-46 |
| End | | 412 | 411 | 503 | 413 | 506 | 220 | 411 | 416 | 210 |
| Start | | 13 | 21 | 225 | 235 | 21 | 21 | 20 | 24 | 21 |
| Chain D | | В | В | a B | Ħ | ٧ | н | н | E | н |
| 203 CD | | ligy | ligy | <u>£</u> | 1,05 | 11mk | E E | lmc o | lmc o | lmc p |
| SEQ No: | | 846 | 846 | 846 | 846 | 846 | 846 | 846 | 846 | 846 |

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|------------------|--------|---|------------------------|------------------|------------------------|-----------------------|-----------------------------|-------------------------------------|--------------------------------------|-------------------------|-----------------------------|-------------------------------|-----------------------|-----------------------------|-----------------------------|-----------------------------|---------------------------------|------------------------------|---|--------------------------|-------------------------------|--|-----------|--------------------|-----------------------------|------------------------------|
| PDB annotation | | CELL ADHESION PROTEIN CELL ADHESION PROTEIN, RGD, EXTRACELLULAR MATRIX, 2 HEPARIN-BINDING, GLYCOPROTEIN | | | , | COMPLEX | (IMMUNORECEPTOR/IMMUNOGLOBU | (IMMUNORECEPTOR/IMMUNOGLOBU LIN) | IMMUNOGLOBULIN IMMUNOGLOBULIN | IMMUNOGLOBULIN VARIABLE | HEAVY (VH) DOMAIN, VARIABLE | LIGHT (VL) ANTIBODY FRAGMENT, | MULTIVALENT ANTIBODY, | DIABODY, DOMAIN 2 SWAPPING, | STRUCTURAL PROTEIN INTEGRIN | HEMIDESMOSOME, FIBRONECTIN, | CARCINOMA, STRUCTURAL 2 PROTEIN | STRUCTURAL PROTEIN INTEGRIN, | HEMIDESMOSOME, FIBRONECTIN, CARCINOMA, STRUCTURAL 2 PROTEIN | IMMUNE SYSTEM FAB, PORA, | NEISSERIA MENINGITIDIS, PORIN | | | IMMUNOGLOBULIN | FV, ANTI-CARCINOEMBRYONIC 2 | STRUCTURAL PROTEIN TENASCIN, |
| Coumpound | 1MCP 4 | FIBRONECTIN; CHAIN: NULL; | IMMUNOGLOBULIN IGG JEL | 103 FAB FRAGMENT | INOSINE-5'-DIPHOSPHATE | NIS ALPHA-BETA T-CELL | RECEPTOR; CHAIN: A, B, C, | н | NIG9 (IGG1=LAMBDA=); CHAIN: 1, H: | SINGLE-CHAIN ANTIBODY | FRAGMENT; CHAIN: A, C; | | | | INTEGRIN BETA 4 SUBUNIT: | CHAIN: A, B; | | INTEGRIN BETA-4 SUBUNIT; | CHAIN: A, B; | ANTIBODY; CHAIN: H, L; | PROTEIN G-PRIME; CHAIN: | A; MAJOR COLLER MEMBRANE PROTEIN PL 16: | CHAIN: P; | MFE-23 RECOMBINANT | CHAIN: A; | TENASCIN; CHAIN: A, B; |
| SeqFold score | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.15 | -0.06 | | | -0.05 | | | 0.13 | 0.04 | | | | | 0.21 | | | 0.24 | | -0.01 | | | | 0.25 | | 0.19 |
| Verify | | -0.03 | 0.05 | | | 0.05 | | | 0.14 | -0.11 | | | | | 0.08 | | | 0.1 | | 0.12 | | | | 0.24 | | 0.04 |
| PSI- BLAST | | 3.60E-21 | 9.60E-64 | | | 4.80E-62 | | | 1.60E-63 | 3.20E-43 | | | | | 5.40E-15 | | | 1.80E-23 | | 3.20E-63 | | | | 8.00E-40 | | 5.40E-19 |
| End | | 715 | 220 | | | 220 | | | 220 | 206 | | | | | 599 | | | 715 | | 220 | | | | 211 | | 713 |
| Start AA | | 512 | 21 | | | 21 | | | 21 | 21 | | | | | 449 | | | 208 | | 21 | | | | 21 | | 512 |
| Chain D | | | H | | | t. | | | Н | V | | | | | V | | | ¥ | | н | | | | V | | A |
| PDB ID | | 뺼 | Imrd | | | Infd | | | Ingp | Indb | | | | | 1gg3 | 1 | | fgpl | | lqkz | | | | Iqok | | lqr4 |
| SEQ NO: D | | 846 | 846 | | | 846 | | | 846 | 846 | | | | | 846 | | | 846 | | 948 | | | | 846 | | 846 |

| PDB annotation | FIBRONECTIN TYPE-III, HEPARIN, EXTRACELLULAR 2 MATRIX, ADHESION, FUSION PROTEIN, STRUCTURAL PROTEIN | CELL ADHESION PROTEIN VCAM- D1,2; 1VCA 6 IMMUNOGLOBULIN SUPERFAMILY, INTEGRIN-BINDING | COMPLEX (ANTIBODY/ELECTRON TRANSPORT) FAB BE, CYTC, ANTIGEN; IMMUNOGLOBULIN, 1GG1 KAPA, FAB FRAGMENT, HORSE 2 CYTOCHRONEC, COMPLEX (AYTIBODY/ELECTRON TRANSPORT) | IMMUNOGLOBULIN ANTI- NITROPHENOL, LAMBDA LIGHT CHAIN, IMMUNOGLOBULIN | CELL ADHESION ICAM-2; IMMUNOGLOBULIN FOLD, CELL ADHESION, GLYCOPROTEIN, 2 TRANSMEMBRANE, REPEAT, SIGNAL | IMMUNE SYSTEM PS8 NATURAL KILLER CELL RECEPTOR; KIR, NATURAL KILLER RECEPTOR, INHIBITORY RECEPTOR, 2 IMMUNOGLOBULIN | | IMMUNE SYSTEM CD32; RECEPTOR, FC, CD32, IMMUNE SYSTEM | IMMUNE SYSTEM CD32; RECEPTOR, FC, CD32, IMMUNE SYSTEM | | ENDOCYTOSIS/EXOCYTOSIS NSECI; PROTEIN-PROTEIN COMPLEX, |
|------------------|--|---|--|--|--|---|--|--|---|--|---|
| Coumpound | | HUMAN VASCULAR CELL ADHESION MOLECULE-1; 1VCA 4 CHAIN: A, B; 1VCA 5 | E8 ANTBODY; CHAIN: I, H; CYTOCHROME C; CHAIN: F; | FAB FRAGMENT, CHAIN: NULL; | INTERCELLULAR ADHESION MOLECULE-2; CHAIN: NULL; | MHC CLASS I NK CELL RECEPTOR PRECURSOR; CHAIN: A; | IMMUNOGLOBULIN IG*A FAB FRAGMENT (1539) (GALACTAN-BINDING) 2FBJ 3 | FC GAMMA RIIB; CHAIN: A; | FC GAMMA RIIB; CHAIN: A; | IMMUNOGLOBULIN FAB FRAGMENT FROM HUMAN IMMUNOGLOBULIN IGGI (LAMBDA, HIL) 8FAB 3 | SYNTAXIN BINDING PROTEIN 1; CHAIN: A; |
| SeqFold score | | | | | | | | | | | |
| PMF | | 0.74 | -0.14 | -0.15 | 60:0 | 60.0 | 0.19 | 0.81 | 0.21 | 0 | 0.11 |
| Verify score | | 0.19 | 0.09 | 0 | 0 | 0.29 | 0.12 | 0.13 | -0.04 40.04 | -0.35 | 0.05 |
| PSI- BLAST | | 3.60E-24 | 8.00E-50 | 8.00E-53 | 1.80E-34 | 7.20E-28 | 3.20E-50 | 7.20E-36 | 9.00E-29 | 9.60E-28 | 1.60E-09 |
| End AA | | 319 | 413 | 602 | 326 | 320 | 210 | 323 | 410 | 407 | 480 |
| Start | | 137 | 236 | 419 | 135 | 134 | 21 | 135 | 226 | 234 | 299 |
| Chain TD | | ¥ | н | æ | | v | Н | V | V | ۷ | æ |
| FDB CD | | lvca | lwej | lydh | lzxd | 2dli | 2fbj | 2fcb | 7tcb | 8fab | 1dh1 |
| SEQ B Si | | 846 | 846 | 846 | 846 | 846 | 846 | 846 | 846 | 846 | 847 |

| | _ | _ | | | | | | _ | _ | | _ | | | _ | _ | _ | | | | _ | | | _ | | | _ | | | | | | | _ | _ |
|-----------------|------------------------|---|-----------------------------|--------------------------------------|--|--|--------------------------------------|--------------------------------------|-----------|---------------------|---------|----------------------|---------------------------|--------|-----------------------|------------------|----------------------|------------------------------|---|-----------------------|----------------|----------------------|----------------------------|-----------------------|-----------------|------|--|----------------------|--------------------|------------------------|------------------------|-----------------------|--------|---------------------|
| PDB annotation | MULTI-SUBUNIT | | HYDROLASE BETA-ALPHA BARREL | ANTIMICROBIAL PROTEIN DISULFIDE-RICH | HYDROLASE HYDROLASE, CHITIN DEGRADATION | HYDROLASE HYDROLASE, CHITIN DEGRADATION | HYDROLASE BETA-ALPHA (TIM) BARREL | HYDROLASE BETA-ALPHA (TIM) BARREL | | | | | | | | | | | | | | | | | | | • | | | | | | | |
| Coumpound | SYNTAXIN 1A; CHAIN: B; | | CHITINASE 1; CHAIN: A; | TACHYCITIN; CHAIN: A | CHITINASE B; CHAIN: A, B; | CHITINASE B; CHAIN: A, B; | CHITINASE A; CHAIN: A; | CHITINASE A; CHAIN: A; | HYDROLASE | (GLUCOSIDASE) ENDO- | BETA-N- | ACETYLGLUCOSAMINIDAS | EH, ENDO H (E.C.3.2.1.96) | 1EDT 3 | HYDROLASE(GLUCOSIDASE |) ENDO-BEI A-in- | ACELYLGLUCOSAMINIDAS | E FI (E.C.3.2.1.90) ZEBN 3 · | (ENDOGLYCOSIDASE F1, ENDO F1) 2EBN 4 | HYDROLASE(GLUCOSIDASE |) ENDO-BETA-N- | ACETYLGLUCOSAMINIDAS | E F1 (E.C.3.2.1.96) 2EBN 3 | (ENDOGL YCOSIDASE FI. | ENDO F1) ZEBN 4 | | DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN | (HOMEODOMAIN) MUTANT | WITH CYS 39 1AHD 3 | REPLACED BY SER (C39S) | COMPLEX WITH DNA (NMR, | IAHD 4 16 STRUCTURES) | 1AHD 5 | DNA-BINDING PROTEIN |
| SeqFold | | | | | | | | | | | | | | | | | | | | | | | | | | - | 77.33 | | | | | | | |
| PMF | | | _ | -0.09 | _ | _ | _ | _ | 0.13 | | | | | | 90.0 | | | | | 0.77 | | | | | 1 | | | | | | | | | 1 |
| Verify score | | | 0.35 | 0.19 | 0.47 | 0.51 | 0.41 | 0.33 | -0.15 | | | | | | 0.25 | | | | | -0.3 | | | | | | | | | | | | | | 0.13 |
| PSI- BLAST | | | 4.80E-63 | 1.60E-10 | 1.10E-81 | 1.60E-59 | 3.60E-79 | 9.60E-70 | 4.80E-05 | | | | | | 7.20E-51 | | | | | 0.0067 | | | | | | 2000 | 7.20E-33 | | | | | | | 6.40E-29 |
| End | | | 297 | 367 | 265 | 566 | 281 | 260 | 146 | | | | | | 504 | | | | | ш | | | | | Ī | į | 35. | | | | | | т | 337 |
| Start | | | 2 | 323 | _ | 2 | 1 | 4 | 4 | | | | | | _ | | | | | 4 | | | | | | 1 | 784 | | | | | | | 286 |
| Chain E | | | V | < | A | A | A | ٧ | | | | | | | | | | | | | | | | | | , | <u>.</u> | | | | | | 1 | ~ |
| PDB UD | | | 1d2k | Ide | 1.00 E+15 | 1.00 E+15 | ledq | ledq | ledt | | | | | | Sebn | | | | | 2ebn | | | | | 1 | 1 | and | | | | | | 1 | Page |
| SEO SE | į | | 848 | 848 | 848 | 848 | 848 | 848 | 848 | | | | | | 848 | | | | | 848 | | | | | I | 5 | 84y | | | _ | | | _ | 849 |

| PDB annotation | | | PROTEIN/DNA HOMEODOMAIN, DNA, COMPLEX, DNA-BINDING PROTEIN, PROTEIN/DNA | PROTEINDNA HOMEODOMAIN, DNA, COMPLEX, DNA-BINDING PROTEIN, PROTEINDNA | TRANSCRIPTIONDNA ULTRADINORA; PRE ROTEIN; DNA BINDING, HOMEDODMAIN, HOMEOTIC PROTEINS, DEVELORMENT, 2 SPECIFICITY | TRANSCRIPTIONDNA ULTRABIHORAX; PRAY ROTEIN; DNA BINDING, HOMEDOMAIN, HOMEOTIC PROTEINS, DEVELOPMENT, 2 SPECIFICITY | TRANSFERASE DINUCLEOTIDE- BINDING MOTIF, PHOSPHORIBOSYL TRANSFERASE | |
|------------------|---|---|--|--|---|--|---|---|
| Coumpound | ANTENNAPEDIA PROTEIN (HOMEDODMAND) MUTANT WITH CYS 39 IAHD 3 REPLACED BY SER (C39S) COMPLEX WITH DNA (MMR, IAHD 4 I6 STRUCTURES) | DINA-BINDING PROTEIN ANTENNA-PEDIA PROTEIN (HOMEDOMARI) MUTANT WITH CYS 31 AHD 3 REPLACED BY SER (C39S) COMPLEX WITH DNA (NMR, 1 AHD 4 16 STRUCTURES) 1 AHD 5 | HOMEOBOX PROTEIN HOX- B1; CHAIN: A; PBX1; CHAIN: B; DNA CHAIN: D; DNA CHAIN: E; | HOMEOBOX PROTEIN HOX- BI; CHAIN: A; PBXI; CHAIN: B; DNA CHAIN: D; DNA CHAIN: E; | ULTRABITHORAX HOMEOTIC PROTEIN IV; CHANN A; HOMEOBOX PROTEIN EXTRADENTICLE; CHANN: B; DNA (5'- CHAIN: C; DNA (5'- CHAIN: D; | ULTRABITHORAX HOMEOTIC PROTEIN IV; CHANN A; HOMEOBOX PROTEIN EXTRADENTICLE; CHANN: B; DNA (5'- CHAIN: C; DNA (5'- CHAIN: D; | NICOTINATE MONONUCLEOTIDE:5,6- CHAIN: A; | DNA-BINDING FUSHI TARAZU PROTEIN (HOMEODOMAIN) (NMR, 20 |
| SeqFold score | | | 62.11 | | 65.54 | | | 68.94 |
| PMF | | - | | - | | 66'0 | 61.0- | |
| Verify score | | -038 | | -0.08 | | -0.11 | 0.15 | |
| PSI- BLAST | | 7.20E-33 | 5.40E-32 | 5.40E-32 | 5.40E-31 | 5.40E-31 | 7.20E-11 | 1.30E-27 |
| End | | 351 | 346 | 346 | 342 | 342 | 238 | 351 |
| Start AA | | 286 | 274 | 286 | 285 | 286 | 35 | 283 |
| Chain ID | | e. | · V | v | ∢ | ∢ | ∢ | |
| PDB ID | | lahd | 1672 | 1672 | 1881 | 168i | 1d0s | 1ftz |
| SEQ NO: | | 849 | 849 | 849 | 849 | 849 | 849 | 849 |

| PDB annotation | | | | | | · | | | | | | COMPLEX (DNA-BINDING PROTEIN/DNA) HD; HOMEODOMAIN, | COMPLEX (UNA-BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) HD: HOMEODOMAIN | COMPLEX (DNA-BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING |
|------------------|--------------------|--|--|---|---|---|---|---|---|--------------------|--|---|--------------------------------------|--|--------------------------------------|-----------------------|
| Coumpound | STRUCTURES) IFTZ 3 | DNA-BINDING FUSHI TARAZU PROTEIN (HOMEODOMAIN) (NMR, 20 STRI ICTI IBFS), 1FT7 3 | DNA-BINDING PROTEIN OCT-1 (POU DOMAIN) 10CT | DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN (HOMEODOMAIN) MUTANT WITH CYS 39 1SAN 3 | REPLACED BY SER AND RESIDUES 1-6 DELETED (C39S,DEL 1-6) ISAN 4 (NMR, 20 STRUCTURES) ISAN 5 | DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN (HOMEODOMAIN) MUTANT | WITH CYS 39 ISAN 3 REPLACED BY SER AND | RESIDUES 1-6 DELETED (C39S,DEL 1-6) ISAN 4 (NMR, 20 STR I (CTI IRES) ISAN 5 | DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN | WITH CYS 39 ISAN 3 | RESIDUES 1-6 DELETED (C39S,DEL 1-6) ISAN 4 (NMR, 20 STRUCTURES) ISAN 5 | ANTENNAPEDIA PROTEIN; CHAIN: A, B; DNA; CHAIN: C, | L, E, F, | ANTENNAPEDIA PROTEIN; CHAIN; A. B. DNA: CHAIN; C. | D, E, F, | ANTENNAPEDIA PROTEIN; |
| SeqFold score | | | | 72.13 | | | | | | | | | | 90'69 | | |
| PMF | | 0.84 | 0.12 | | | _ | | | _ | | | | | | | |
| Verify | | -0.31 | -0.2 | | | -0.21 | | | -0.2 | | | 0.11 | | | | 0.27 |
| PSI- BLAST | | 1.30E-27 | 7.20E-34 | 5.40E-30 | | 1.40E-26 | | | 5.40E-30 | | | 1.30E-27 | | 9.00E-30 | | 9.00E-30 |
| End | | 337 | 344 | 351 | | 337 | | | 351 | | | 337 | | 344 | | 344 |
| Start AA | | 284 | 205 | 290 | | 291 | | | 292 | | | 289 | | 289 | | 289 |
| Chain ID | | | ၁ | | | | | | | | | A | | ¥ | | Ą |
| EDB DD | | 1#2 | - ö | Isan | | Isan | | | Isan | | | 9ant | | 9ant | | 9ant |
| SEQ NO: | | 849 | 849 | 849 | | 849 | | | 849 | | | 849 | | 849 | | 849 |

| PDB annotation | PROTEIN/DNA) HD; HOMEODOMAIN, COMPLEX (DNA-BINDING PROTEIN/DNA) | COMPLEX (TRANSMEMBRANE/GLYCOPROTEIN) MHC GLYCOPROTEIN, COMPLEX | (TRANSMEMBRANE/GLYCOPROTEIN) COMPLEX (TRANSMEMBRANE/GLYCOPROTEIN) MHC GLYCOPROTEIN, COMPLEX (TRANSMEMBRANE/GLYCOPROTEIN) | COMPLEX (MHC PROTEIN/ANTIGEN) DRA, DRBI 01010; COMPLEX (MHC PROTEIN/ANTIGEN), HISTOCOMPATIBILITY ANTIGEN | COMPLEX (MHC PROTEINVANTIGEN) DRA, DRBI 01010, COMPLEX (MHC PROTEIN/ANTIGEN), HISTOCOMPATIBILITY ANTIGEN | IMMUNE SYSTEM HIA-DR2, MYELIN BASIC PROTEIN, MULTIPLE SCLEROSIS, 2 AUTOIMMUNITY, IMMUNE SYSTEM | IMMUNE SYSTEM HLA-DR2, MYELIN BASIC PROTEIN, MULTIPLE SCLEROSIS, 2 AUTOIMMUNITY, IMMUNE SYSTEM | NACHA-DOK-HA-ADK-HA-DOK-HA-DOK-HA-DOK-HA-ADK-HA-DOK-BOW-EX-YOM-EX-YOM-EX-YOM-EX-YOM-EX-YOM-EX-YOM-EX-YOM-EX-YOM-BOW-HA-DOK-HA-DO | IMMUNE SYSTEM MHC CLASS II DR2A |
|------------------|---|--|--|--|--|---|---|--|------------------------------------|
| Coumpound | CHAIN: A, B; DNA; CHAIN: C, D, E, F; | HLA-DR3; CHAIN: A, B; CLIP; CHAIN: C; | HLA-DR3; CHAIN: A, B; CLIP; CHAIN: C; | HLA-DRI CLASS II HISTOCOMPATIBILITY PROTEIN; CHAIN: A, B, D, E, G, H, J, K; HLA-A2; CHAIN: C, F, I, L; | HLA-DRI CLASS II HISTOCOMPATIBILITY PROTEIN: CHAIN: A, B, D, E, G, H, J, K; HLA-A2; CHAIN: C, F, I, L: | HLA-DR2; CHAIN: A, D; HLA- DR2; CHAIN: B, E; HLA-DR2; CHAIN: C, F; | HLA-DR2; CHAIN: A, D; HLA- DR2; CHAIN: B, E; HLA-DR2; CHAIN: C, F; | HIA CLASS II HISTOCOMATIBILITY ANTIGER: CHAIN: A; HLA CLASS II HISTOCOMPATIBILITY ANTIGER: CHAIN: B; ENTEROTOXIN TYPE B; CHAIN: CPETIBE CHAIN: CHAIN: D; | MAJOR HISTOCOMPATIBILITY |
| SeqFold score | | 54.43 | | | 55.9 | | 52.4 | | |
| PMF | | | 0.93 | 0.63 | | 0.87 | | 0.92 | 0.82 |
| Verify | | | -0.32 | -0.33 | | -0.22 | | -0.33 | -0.31 |
| PSI- BLAST | | 3.20E-66 | 3.20E-66 | 6.40E-69 | 6.40E-69 | 1.60E-69 | 1.60E-69 | 4.80E-62 | 3.20E-67 |
| End | | 157 | 147 | 147 | 157 | 147 | 157 | 147 | 147 |
| Start AA | | 33 | 34 | 33 | 8 | 32 | 32 | 31 | 30 |
| Chain | | щ | æ | æ | æ | В | æ | m | В |
| 10B CD | | Ia6a | Ia6a | laqd | laqd | lbx2 | Ibx2 | 145 E | 14vI |
| S e S | | 851 | 821 | 821 | 821 | 821 | 821 | 851 | 821 |

| PDB annotation | | HISTOCOMPATIBILITY ANTIGEN I-AK HISTOCOMPATIBILITY ANTIGEN, MHC. PEPTIDE COMPLEX | MHC II MHC II, CLASS II MHC, I-A, OVALBUMIN PEPTIDE | MHC II MHC II, CLASS II MHC, I-A, OVALBUMIN PEPTIDE | HISTOCOMPATIBILITY ANTIGEN HISTOCOMPATIBILITY ANTIGEN | HISTOCOMPATIBILITY ANTIGEN HISTOCOMPATIBILITY ANTIGEN | HISTOCOMPATIBILITY ANTIGEN HISTOCOMPATIBILITY ANTIGEN | MHC II MHC II, CLASS II MHC I-AD | MHC II MHC II, CLASS II MHC I-AD | BLOOD COAGULATION BLOOD COAGULATION, EGF, HYDROLASE, SERINE PROTEASE | STRUCTURAL PROTEIN INTEGRIN- BINDING PROTEIN, INV GENE | | BLOOD COAGULATION, SERINE PROTEASE, COMPLEX, CO-PACTOR, 2 RECEPTOR ENZYME, INHIBITOR, GLA, EGF, 3 COMPLEX (SERINE PROTEASE/COFACTOR/LIGAND) | |
|------------------|--|--|--|--|---|---|---|------------------------------------|------------------------------------|--|---|--|---|--|
| Coumpound | COMPLEX ALPHA CHAIN; CHAIN; A, D; MAJOR HISTOCOMPATIBILITY COMPLEX BETA CHAIN; CHAIN; B, E, MYELIN BASIC PROTEIN; CHAIN; C, F; | MHC CLASS IIT-AK; CHAIN: A, B, P; HEN EGGWHITE LYSOZYME PEPTIDE | MHC CLASS II I-AD; CHAIN: A, B; | MHC CLASS II I-AD; CHAIN: A, B; | MHC CLASS II I-EK; CHAIN: A, B, C, D; | MHC CLASS II I-EK; CHAIN: A, B, C, D; | MHC CLASS II I-EK; CHAIN: A, B, C, D; | MHC CLASS II I-AD; CHAIN: A, B; | MHC CLASS II I-AD; CHAIN: A, B; | FACTOR VII; CHAIN: NULL; | INVASIN; CHAIN: A; | GLYCOSYLTRANSFERASE CYCLODEXTRIN GLUCANOTRANSFERASE (E.C.2.4.1.19) (CGTASE) 1CYG 3 | BLOOD COAGULATION FACTOR VIIA; CHAIN: I., H; SOLUBLE TISSUE FACTOR; CHAIN: T, U; D-PHE-PHE- ARG. | CHLUKUME I HYLKETONE (DFFRCMK) WITH CHAIN: C, |
| SeqFold score | | | 52.61 | | | 50.29 | | 52.73 | | | | | | |
| PMF | | 0.46 | | 0.71 | 6.0 | | 0.87 | | _ | 0.17 | -0.19 | -0.19 | 0.04 | |
| Verify | | -0.4 | | -0.39 | -0.27 | | -0.43 | | -0.5 | -0.42 | 0.05 | 0.07 | -0.24 | |
| PSI- BLAST | | 4.80E-53 | 9.60E-57 | 9.60E-57 | 1.40E-63 | 1.40E-63 | 8.00E-64 | 3.20E-58 | 3.20E-58 | 0.0072 | 3.60E-19 | 7.20E-15 | 0.009 | |
| End | | 147 | 157 | 147 | 147 | 157 | 147 | 157 | 147 | 474 | 229 | 226 | 475 | |
| Start AA | | 36 | 23 | 35 | 29 | ∞ | 24 | 77 | 56 | 443 | 2 | 17 | 404 | |
| Chain ID | | В | В | В | В | ш. | В | В | В | | ٧ | | J | |
| PDB ID | | liak | liao | Iiao | liea | liea | lieb | 2iad | 2iad | 1669 | lcwv | lcyg | Idan | |
| SEQ NO: | | 851 | 158 | 851 | 821 | 851 | 821 | 158 | 851 | 856 | 826 | 826 | 826 | |

| PDB annotation | HYDROLASEHYDROLASE INHIBITOR PROTEIN-PEPTIDE COMPLEX | HYDROLASE NEURAMINIDASE; HYDROLASE, GLYCOSIDASE | BLOOD CLOTTING FACTOR VII, BLOOD COAGULATION, EGF-LIKE DOMAIN, BLOOD 2 CLOTTING | GROWTH FACTOR NEU DIFFERENTIATION FACTOR (RAT), ACETYLCHOLINE GROWTH FACTOR | | GLYCOSYLTRANSFERASE TRANSFERASE, GLYCOSYLTRANSFERASE, CALCIUM, SIGNAL | | HYDROLASE HYDROLASE, LIPID DEGRADATION, PANCREATIC LIPASE | HYDROLASE HYDROLASE, LIPID DEGRADATION, PANCREATIC LIPASE | COMPLEX (HYDROLASE/COFACTOR) TRIACYLGLYCEROL LIPASE; COMPLEX (HYDROLASE/COFACTOR), LIPID DEGRADATION | COMPLEX (HYDROLASE/COFACTOR) TRIACYLGLYCEROL LIPASE; COMPLEX (HYDROLASE/COFACTOR), LIPID DEGRADATION |
|------------------|---|--|---|---|--|--|---|--|--|--|--|
| Coumpound | DES-GIA FACTOR VIIA HERAYY CHAND; CHAND; HAND; C, D; PEPTIDE E-76; CHAND; X; Y; | SIALIDASE; CHAIN: NULL; | BLOOD COAGULATION FACTOR VII; CHAIN: A; | HEREGULIN-ALPHA; CHAIN: NULL; | GROWTH FACTOR HEBGGULN-ACLHAA (EPIDERAAL GROWTH FACTOR-LIKE DOMAIN) HTRE 3 (NMX, MINIMIZED AVERAGE STRUCTURE) HTRE 4 | CYCLODEXTRIN GLUCANOTRANSFERASE; CHAIN: A, B; | | PANCREATIC LIPASE RELATED PROTEIN 2; CHAIN: A; | PANCREATIC LIPASE RELATED PROTEIN 2; CHAIN: A; | TRIACYLGI YCEROL ACYL- HYDROLASE; CHAIN: A, C; COLIPASE; CHAIN: B, D | TRIACYLGLYCEROL ACYL. HYDROLASE; CHAIN: A, C; COLIPASE; CHAIN: B, D |
| SeqFold score | | | | | | | | | | 167.54 | |
| PMF | 0.28 | -0.19 | 0.11 | 0 | 0.23 | -0.19 | | | _ | | _ |
| Verify score | 0.07 | 0.22 | -0.28 | -0.21 | -0.7 | 0.04 | | 0.85 | 0.81 | | 0.65 |
| PSI- BLAST | 0.0036 | 7.20E-13 | 0.0036 | 0.0072 | 0.0072 | 5.40E-12 | | 3.60E-83 | 4.80E-65 | 1.60E-66 | 1.60E-66 |
| End | 472 | 232 | 475 | 482 | 254 | 171 | | 256 | 276 | 276 | 276 |
| Start | 429 | 81 | 443 | 429 | 230 | | | 18 | 82 | 18 | 18 |
| Chain ID | د | | 4 | | | ∢ | | ٧ | ¥ | ∢ . | ∀ |
| EGA ED | Idva | ja j | 1f7e | Ihae | -th | n m | - | 1bu8 | 1bu8 | leth | leth |
| S e S | 856 | 826 | 928 | 856 | | 826 | 1 | 857 | 857 | 857 | 857 |

| | , | | | , | | | , |
|------------------|--|---|---|---|---|--|---|
| PDB annotation | SERINE ESTERASE RELATED PROTEIN 2 LIPASE; SEBINE ESTERASE, HYDROLASE, IPID DEGRADATION, PANCREAS, 2 GLYCOPROTEIN, CHIMERIC | SERINE ESTERASE RELATED PROTEIN 2 LIPASE; SERINE ESTERASE, HYDROLASE, LIPID DEGRADATION, PANCREAS, 2 GLYCOPROTEIN, CHIMERIC | SERINE ESTERASE RELATED PROTEIN 2 LIPASE; SERINE ESTERASE, HYDROLASE, ILPID DEGRADATION, PANCREAS, 2 GLYCOPROTEIN, CHIMERIC | | | | |
| Coumpound | RP2 LIPASE; CHAIN: NULL; | RP2 LIPASE; CHAIN: NULL; | RP2 LIPASE; CHAIN: NULL; | HYDROLASE(CARBOXYLIC ESTERASE) LIPASE (E.C.3.1.1.3) (TRIACYLGLYCEROL HYDROLASE) 1HPL3 | HYDROLASE/CARBOXYLIC ESTRRASD, ILPASE (E.C.3.1.1.3) COMPLEXED WITH COLIFASE AND NHBITED ILPB 3 BY UNDECANE PHOSPHONATE WEITHYL ESTRE (TWO CONFORMATIONS) ILPB 4 | HYDROLASE(CARBOXYLIC SETREASE) LIPASIE (E.C.3.11.3) COMPLEXED WITH COLIPASE AND INHIBITED ILPB 3 BY MUNDECANE PHOSPHONATE METHYL ESTER (TWO COMPORMATIONS) ILPB 4 | HYDROLASE(CARBOXYLIC ESTERASE) LIPASE (E.C.3.1.1.3) COMPLEXED WITH COLIPASE AND NHIBITED 11.PB 3 BY |
| SeqFold score | 176.81 | | | 167 | | 173.41 | |
| PMR | | - | _ | | | | _ |
| Verify score | | 0.87 | 0.76 | | 0.83 | | 0.81 |
| PSI- BLAST | 1.80E-80 | 1.80E-80 | 3.20E-65 | 1.60E-76 | 1.10E-79 | 1.10E-79 | 1.60E-65 |
| End | 276 | 256 | 276 | 274 | 256 | 276 | 276 |
| Start | 18 | 61 | 19 | 18 | 81 | 18 | 18 |
| Chain ID | | | | | æ | æ | B |
| PDB ID | lgg1 | lgg! | lga! | Ihpl | 11pb | 11pb | 1lpb |
| SEQ NO: | 857 | 857 | 857 | 857 | 857 | 857 | 857 |

| | | | | | - | | | Т | | | | T- | | _ | _ | _ | $\overline{}$ | _ | _ | |
|------------------|--|--|--|--|---|--|---|-----------------------|--|--|--|-------------------|--|--------------------------|------------------------|-----------------------|-------------------|----------------------------|--------------------------|---|
| PDB annotation | | HYDROLASE HYDROLASE, LIPID DEGRADATION, PANCREATIC LIPASE | HYDROLASE HYDROLASE, LIPID DEGRADATION, PANCREATIC LIPASE | HYDROLASE HYDROLASE, LIPID DEGRADATION, PANCREATIC LIPASE | | ENDOCYTOSIS/EXOCYTOSIS NSECI; PROTEIN-PROTEIN COMPLEX, MULTI-SUBUNIT | TRANSCRIPTION INHIBITOR BETA- PROPELLER | CONTRIBE CONTRIBUTION | COMPLEA (917- BINDING/TRANSDUCER) BETA1, TRANSDUCN BETA SUBLINE. | GAMMAI, TRANSDUCIN GAMMA SUBUNIT; COMPLEX (GTP- | BINDING/TRANSDUCER), G PROTEIN, HETEROTRIMER 2 SIGNAL TRANSDUCTION | COMPLEX (GTP- | BINDING/TRANSDUCER) BETA1, TRANSDUCIN BETA STREEN.T. | GAMMAI, TRANSDUCIN GAMMA | SUBUNIT; COMPLEX (GTP- | HETEROTRIMER 2 SIGNAL | COMPLEX (GTP- | BINDING/TRANSDUCER) BETA1, | GAMMAI TRANSDICTOR GAMMA | SUBUNIT; COMPLEX (GTP-BINDING/TRANSDUCER), G PROTEIN, |
| Coumpound | UNDECANE PHOSPHONATE METHYL ESTER (TWO CONFORMATIONS) 1LPB 4 | PANCREATIC LIPASE RELATED PROTEIN 1; CHAIN: NULL; | PANCREATIC LIPASE RELATED PROTEIN 1; CHAIN: NULL; | PANCREATIC LIPASE RELATED PROTEIN 1; CHAIN: NULL; | | SYNTAXIN BINDING PROTEIN 1; CHAIN: A; SYNTAXIN 1A; CHAIN: B; | TRANSCRIPTIONAL REPRESSOR TUP1; CHAIN: A, B. C; | OT ATPITATOL ALDITA | CHIMERA; CHAIN: A; GT- | GAMMA; CHAIN: G; | | GT-ALPHA/GI-ALPHA | CHIMERA: CHAIN: A; GT- | GAMMA; CHAIN: G; | | | GT-ALPHA/GI-ALPHA | CHIMERA; CHAIN: A; GT- | GAMMA CHAIN: B; GI- | () |
| SeqFold score | | | 183.05 | | | | | | | | | 52.34 | | | | | | | | |
| PMF | | 1 | | - | | 0 | 0.07 | 5 | 7 7 | | | | | | | | -0.11 | | | |
| Verify | | 69:0 | | 0.71 | | -0.08 | 0.28 | 250 | 9.19 | | | L | | | | | 0.13 | | | |
| PSI- BLAST | | 5.40E-83 | 5.40E-83 | 1.60E-63 | | 0.00036 | 1.30E-44 | 27 200 0 | 9:002-40 | | | 1.10E-40 | | | | | 1.10E-40 | | | |
| End | | 257 | 274 | 276 | | 156 | 308 | 900 | 967 | | | 309 | | | | | 309 | | | |
| Start | | 18 | 81 | 18 | | 14 | 151 | 133 | 76 | | | « | | | | | 95 | | | |
| Chain | | | | | | g | ¥ | l. | ۵ | | | В | | | | | В | | | |
| PDB DD | | lq1 | Iqil | Īģ. | | Idhl | lej. | 1 | 1091 | • | | lgot | | | | | Igot |) | | |
| SEQ NG B G | | 857 | 857 | 857 | | 628 | 829 | 050 | ŝ | | | 829 | | | | | 829 | | | |

| | | | | | | | 8 | | | |
|------------------|------------------------------------|---|---|---|---|---|---|---|---|---|
| PDB annotation | HETEROTRIMER 2 SIGNAL TRANSDUCTION | OXIDOREDUCTASE ENZYME, WITKITE REDUCTASE, OXIDOREDUCTASE, DENITREFICATION, 2 ELECTRON TRANSPORT, PERPLASMIC | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGERDNA) COMPLEX (ZINC FINGERDNA), ZINC FINGER, DNA-BINDING PROTEIN | COMPLEX (ZINC FINGERDNA) ZINC FINCER, PROTEIN-DNA, INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERODNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 |
| Coumpound: | | CYTOCHROME CDI NITRITE REDUCTASE, CHAIN: A, B; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE: CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE, CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE: CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN: CHAIN: C, F, G; |
| SeqFold score | | | | | | | | | | |
| PMF | | -0.12 | 0.15 | _ | - | 86.0 | 66.0 | 0.07 | 0.52 | _ |
| Verify score | | 0 | -0.3 | 0.04 | 0.48 | 0.27 | 0.41 | -0.35 | -0.16 | 0.1 |
| PSI- BLAST | | 1.30E-14 | 1.60E-25 | 1.80E-39 | 9.00E-38 | 3.60E-39 | 6.40E-31 | 1.10E-39 | 3.20E-43 | 1.40E-44 |
| End | | 304 | 221 | 277 | 306 | 640 | 640 | 193 | 221 | 249 |
| Start | | 221 | 141 | 197 | 225 | 995 | 260 | 112 | 140 | 168 |
| Chain | | 4 | ¥ | ¥ | ¥ | ∢ | Ą | ပ | ပ | ပ |
| ED CI | | 14ks | lalh | lalh | lalh | lalh | lath | Ime y | Jmc y | lme y |
| SEQ NO: DE | | 658 | 098 | 098 | 098 | 098 | 098 | 098 | 098 | 860 |

| PDB annotation | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX | COMPLEX (ZINC FINGERDNA) ZINC COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA FINGER, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX |
|-----------------|--|---|--|--|--|--|---|--|---|
| Coumpound | | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A. B. D. E. CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; |
| SeqFold | | | | | | | | | |
| PMF | | ı | _ | _ | _ | _ | _ | _ | _ |
| Verify score | | 0.23 | 0.55 | 0.49 | 0.62 | 0.34 | 0.27 | 0.42 | 0.16 |
| PSI- BLAST | | 1.60E-46 | 1.60E-47 | 1.40E-48 | 3.20E-49 | 8.00E-50 | 1.60E-50 | 1.60E-50 | 4.80E-50 |
| End | | 277 | 305 | 333 | 361 | 389 | 417 | 445 | 473 |
| Start | | 196 | 224 | 252 | 280 | 308 | 336 | 364 | 392 |
| Chain | | υ | v | U | U | v | U | U | ပ |
| PDB U | | Jme y | y Jme | y line | Jme y | y y | Jme y | J me | y Jmc |
| ğ a ÿ | | 098 | 098 | 098 | 098 | 098 | 098 | 098 | 098 |

| | | | | | | | _ | _ | | , | | | | _ | | _ | | _ | | _ | | _ | | | | _ | _ | _ | |
|------------------|-------------------|---|-------------------|--------------------------------|--------------------------------|--|--------------------------------|--|----------------------------|--------------------------------|-----------------------|--------------------------------|----------------------------|--------------------|--|--------------------------------|----------------------------|--------------------------------|-----------------------|--------------------------------|--|--------------------------------|-----------------------|--------------------------------|----------------------------|----------------------------------|-----------------------|--------------------------------|--|
| PDB annotation | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | (ZINC FINGER/DINA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | COMPLEX STRICE PRICES TO TRICE | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER/DNA) ZINC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX | COMPLEY (ZBIC ENICER (DAIA) ZBIC | FINGER, PROTEIN-DNA | INTERACTION, PROTEIN DESIGN, 2 | CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) |
| Coumpound | | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | | DNA; CHAIN: A, B, D, E; | PROTEIN; CHAIN: C, F, G; | | DNA; CHAIN: A, B, D, E; | PROTEIN: CHAIN: C. F. G. | | DNA: CHAIN: A. B. D. E. | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | | CONSENSUS ZINC FINGER | PROTEIN, CHAIN: C, F, G; | | PM4. Ollifal. 4 B P. C. | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | | DNA: CUAN: A B D E. | CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; | |
| SeqFold score | | | | | | | | | | | | | | | | | | 101 07 | 0.101 | | | | | | | | | | |
| PMF | | 86.0 | | 1 | | | 96'0 | | | 1 | | | | | | | | | | | | - | | | | - | | | |
| Verify score | | -0.22 | | 0.1 | | | 0.15 | | | 0.43 | ! | | | 9 | 69. | | | | | | | 0.71 | | | | 0.30 | | | |
| PSI- BLAST | | 7.20E-33 | | 9.60E-50 | | | 3.20E-47 | | | 3.20E-47 | | | | 0 707 | 9.60E-50 | | | 0 000 50 | 0.700.0 | | | 8.00E-50 | | | | 1 KOP.40 | 200 | | |
| End | | 200 | | 201 | | | 228 | | | 556 | | | | 705 | 284 | | | 202 | 3 | | | 612 | | | | 640 | Ē | | |
| Start AA | | 392 | | 420 | | | 448 | | | 476 | | | | 2 | 90C | | | 203 | 3 | | | 531 | | | | 640 | } | | |
| Chain ID | | υ_ | | ပ | | | ပ | _ | | S | | | | , | _ د | | | L | | | | ပ | | | | C | | | |
| PDB CD | | y me | | lme ^ | , | | je . | ^ | | Ime | ^ | | | 1 | <u> </u> | | | lme | , × | | | lme | ٨ | | | Ime | _ | | |
| SEQ No: D | | 980 | | 980 | | | 98 | | | 860 | | | | 070 | 2 | _ | | 860 | 3 | | | 99 | | _ | | 860 | } | | |

| PDB annotation | COMPLEX (ZINC FINGERDNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGERDNA) | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (TRANSCRIPTION REGULATIONIDNA) COMPLEX (TRANSCRIPTION REGULATIONIDNA), RNA REGULATIONIDNA), RNA POLYMERASE II, 2 TRANSCRIPTION INITATION, ZNO; PINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONIDNA) COMPLEX (TRANSCRIPTION) REGULATIONIDNA), RNA REGULATIONIDNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZNO, FINGRR PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONIDA) COMPLEX (TRANSCRIPTION) REGULATIONIDA), RNA POLYMEASE II, 2 TRANSCRIPTION INITATION, ZING FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONIDA) COMPLEX REGULATIONIDA), RANSCRIPTION REGULATIONIDAN, RAN POLYMEASE III, 2 TRANSCRIPTION INTIATION, ZINC FINGRR PROTEIN | COMPLEX (TRANSCRIPTION REGULATIONIDNA) COMPLEX (TRANSCRIPTION REGULATIONIDNA), RNA REGULATIONIDNA), RNA POLYMERASE III, 2 TRANSCRIPTION NITTATION, ZNG, ENGRE PROTFIN | COMPLEX (TRANSCRIPTION |
|------------------|--|--|---|--|--|--|---|-------------------------|
| Coumpound | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G; | DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINCER PROTEIN; CHAIN: C, F, G; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA, CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S |
| SeqFold score | | | | | 105.92 | | | |
| PMF | 0.94 | 0.94 | 0.12 | 0.99 | | - | - | 0.99 |
| Verify score | 90.0 | 90:0 | -0.25 | 0.11 | | 0.21 | 0.32 | 0.16 |
| PSI- BLAST | 3.60E-14 | 4.80E-13 | 4.80E-31 | 1.60E-35 | 1.80E-66 | 4.80E-37 | 1.60E-38 | 1.30E-36 |
| End | 333 | 333 | 258 | 314 | 393 | 370 | 426 | 537 |
| Start | 306 | 306 | 113 | 169 | 224 | 225 | 281 | 393 |
| Chain | G | _O | ∢ | ∀ | < | ∢ | ∢ | ٧ |
| 80 a | y me | r Ime | 148 | <u></u> | 1E | 911 | 116 | 3 |
| Se di | 098 | 098 | 098 | 098 | 098 | 098 | 098 | 986 |

| PDB annotation | REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DA), RNA PO! YMERASE III, 2 TRANSCRIPTION INTTATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REQUILATIONIDA) COMPLEX (TRANSCRIPTION REGULATIONIDA), RNA REGULATIONIDA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULT/TONDINA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMEASB III, 2 TRANSCRIPTION INTIA/TION, ZING PINGER PROTEIN INTIA/TION, ZING PINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/ONA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA REGULATION/DNA), RNA ROLYMERSE BILL 3 TRANSCRIPTION INITIATION, ZNO FINGER PROFIEN | COMPLEX TRANSCRIPTION REGULATION/DNA) YING-XANG 1; TRANSCRIPTION INITIATION; INITIATION ELEMENT, YV. I. ZNC.2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX TRANSCRIPTION REGULATION/DNA YING-YANG I; TRANSCRIPTION INITIATION INITIATION ELEMENT YY II. ZNC 2 FINGER PROTEIN, DNA-ROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION) | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-YANG I; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 |
|-----------------|--|---|---|---|---|---|--|
| Coumpound | RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INTIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B; | YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B; |
| SeqFold | | | | | | | |
| PMF | | 0.64 | 0.68 | - | 0 | 0.83 | 69.0 |
| Verify score | | 0.11 | 1.0- | 90.0 | -0.43 | -0.19 | -0.37 |
| PSI- BLAST | | 8.00E-38 | 6.40E-35 | 9.60E-35 | 9.60E-29 | 1.30E-30 | 1.80E-34 |
| End | | 565 | 298 | 929 | 22 | 249 | 277 |
| Start AA | | 421 | 449 | 477 | | 148 | 150 |
| Chain B | | ∢ | ⋖ | ∢ | ပ | U | υ |
| 108 CD | | 911 | 941 | 9311 | Inbd | Iubd | lubd |
| S e S | | 098 | 098 | 098 | 860 | 098 | 098 |

| | NA) | <u>ئ</u> | 7 | NA) | | | | (ANC | | | | _ | | (AVC | | | | 7 | | (AVC | | <u></u> | 2 | _ | (ANC | 011 | -: |
|-----------------|--|---|--|-------------------------------|--|--|-----------------------------|--|------------------------|------------------------------|---------------------------|----------------------------|------------------------|-------------------------------|------------------------|------------------------------|---------------------------|--------------------------------|------------------------|--------------------------------|------------------------|--------------------------|--------------------------------|-----------------------------|---|------------------------|---|
| | FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG I; TRANSCRIPTION INITIATION, | NITIATOR ELEMENT, YYI, ZINC 2 TINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX | TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG I; | TRANSCRIPTION INITIATION, NITIATOR ELEMENT VYI 2INC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX TRANSCRIPTION REGULATION DNA) | NOL | REGULATION/DNA) YING-YANG I; | IKANSCRIPTION INITIATION, | FINGER PROTEIN DNA-PROTEIN | EX | TRANSCRIPTION REGULATION/DNA) | NOI | REGULATION/DNA) YING-YANG I; | TION, | INITIATOR ELEMENT, 111, ZINC 2 | EX | (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION | TION. | INITIATOR ELEMENT, YYI, ZINC 2 | FINGER PROTEIN, DNA-PROTEIN | RECOGNITION, 3 COMPLEX TRANSCRIPTION REGILI ATIONONA) | LON | REGULATION/DNA) YING-YANG 1; IRANSCRIPTION INITIATION, |
| PDB annotation | FINGER PROTEIN, DNA-PRO RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULAT | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YAI TRANSCRIPTION INITIATION, | INITIATOR ELEMENT, YYI, FINGER PROTEIN, DNA-PRC RECOGNITION, 3 COMPLEX | N REGU | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YA | TRANSCRIPTION INITIATION | IN, DNA- | RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULA) | COMPLEX (TRANSCRIPTION | NA) YIN | IKANSCKIPTION INITIATION, | IN DNA | RECOGNITION, 3 COMPLEX | ON REGU | COMPLEX (TRANSCRIPTION | JNA) YIN | TRANSCRIPTION INITIATION, | MENI, I | RECOGNITION, 3 COMPLEX | ON REGU | COMPLEX (TRANSCRIPTION | RANSCRIPTION INITIATION, | MENT, Y | N DNA | RECOGNITION, 3 COMPLEX TRANSCRIPTION REGILLAN | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-YA |
| PDE | REOTEI NITION, SCRIPTIC | EX (TRA ATION/E CRIPTIO | TOR ELE R PROTEI INITION, | SCRIPTIC | ATIONE ATIONE | CRIPTIO TOR FIFE | PROTE | NITTON, SCRIPTIC | EX (TRA | ATIONE | CKIP 110 | A PROTE | NOTTIN'S | SCRIPTIC | EX (TRA | MOLLA | CRIPTIO | D PPOTE | NOLLIN. | SCRIPTIC | LEX (TRA | CRIPTIO | TOR ELE | R PROTE | NOLLINE SCRIPTION, | EX (TR | ATIONI |
| | RECOG (TRAN) | COMPI REGUL TRANS | FINGE | TRAN | REGUL | TRANS | FINGE | RECOC | COMPI | REGUI | IKANS | FINGE | RECOC | (TRAN | COMPI | REGUI | IRAN | FINGE | RECO | (TRAN | COMPI | TRANS | NITIA | FINGE | RECO | COMP | REGUI |
| | | PS DNA: | | 9 | ې گ | DNA; | | | S | P5 | DNA; | | | | -Q. | <u>ج</u> | r DNA; | | | | o z | L DNA: | | | | ģ | PS TONA; |
| Coumpound | | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; | | 1 | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | | | YYI; CHAIN: C; ADENO- | ASSOCIATED VIRUS PS | INITIATOR ELEMENT DNA; | | | | YYI; CHAIN: C; ADENO- | ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | | | | YY1; CHAIN: C; ADENO- | NITIATOR ELEMENT DNA: | | | | YYI CHAIN C. ADENO- | ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; |
| Con | | CHAIN: OCIATEI | CHAIN: A, B; | | CHAIN OCIATEI | INITIATOR EI | 1 | | CHAIN | OCIATE | INITIATOR E | ų, 7, 14 ų | | | ; CHAIN | OCIATE | TATOR | CHAIN: A, B; | | | CHAIN | TATOR | CHAIN: A, B; | | | CHAIN | OCIATE TATOR I |
| _ | - | ASS | 용 | - | ASS | Z S | 3 | | Į. | ASS | 3 8 | 5 | | | 7. | ASS | Z | 5 | _ | _ | λ.λ | 22 | E | | | * | ASS |
| SeqFold | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 0.93 | | | 96.0 | | | | _ | | | | | | - | | | | | | 98.0 | | | | | L | |
| Verify score | | -0.19 | | 100 | -0.02 | | | | 0.19 | | | | | | 0.27 | | | | | | 9.04 | | | | | 0.0 | } |
| PSI- BLAST | | 3.20E-32 | | 6, 200 | 1.80E-48 | | | | 4.80E-34 | | | | | | 3.20E-34 | | | | | | 5.40E-52 | | | | | 3 20F-34 | |
| End | | 277 | | + | 333 | | | | 333 | | | | | | 361 | | | | _ | | 445 | _ | _ | | | 417 | |
| Start | | 170 | | | 194 | | | | 227 | | | | | | 260 | | | | | | 306 | | | | | 316 | 2 |
| Chain | | U | | | U | | | | U | | | | | | J | | | | | | o | | | | | c | , |
| FDB CD | | Inpq | | -+ | P P P | | | | Jubd | | | | | | Jubdu | _ | | | | | Jubd | _ | | | | jpq | 3 |
| SEQ E | Ž | 098 | | | 980 | | | | 098 | | | | | _ | 98 | | | | | _ | 98 | _ | | | | 860 | } |

| | | , | | | | | |
|------------------|--|---|--|--|--|--|--|
| PDB annotation | INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULATIONDAN) TMG-YANO I; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRPTION REQUILATIONDAN) TMG-YAND I; TRANSCRPTION INTIATION, INITIATIOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRPTION REGULATIONDAN) | COMPLEX (TRANSCRPTION REGULATIONIONA) YING-YANG I; TRANSCRPTION INITIATION, INITATIOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX TRANSCRPTION REGULATIONIONA) | COMPLEX (TRANSCRIPTION REQUILATIONDAN) YING-YANG I; TRANSCRIPTION INITIATION, INITIATIOR BLEMBIN, YYI, ZING Z FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDAN) | COMPLEX (TRANSCRIPTION REQUILATIONDAA) YING-YANG 1; TRANSCRIPTION INITIATION, INITATIOR ELEMENT, YY1, ZINO.2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX TRANSCRIPTION REGIT ATTOMANAA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG I: |
| Coumpound | CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED YIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI, CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS NITIATOR ELEMENT DNA; CHAIN: A, B; | YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INTIATOR ELEMENT DNA; CHAIN: A. B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 |
| SeqFold score | | | | | | | |
| PMF | | - | 0.53 | 0.78 | 96.0 | - | L |
| Verify score | | -0.14 | -0.42 | 0 | -0.07 | 0.23 | 0.22 |
| PSI- BLAST | | 4.80E-35 | 3.60E-42 | 6.40E-35 | 3.20E-31 | 1.80E-47 | 3.20E-36 |
| End | | 473 | 256 | · 102 | 226 | 284 | 584 |
| Start | | 372 | | 400 | 456 | 481 | 484 |
| Chain D | | ပ | ပ | υ | υ | ပ | ပ |
| ED (I) | | lubdu . | pqn[| Iubd | lubd | Jubd | Inpq |
| Se o Se | | 860 | 098 | 098 | 098 | 098 | 98 |

| | | | | | | | | , |
|------------------|---|---|--|--|--|--|---|--|
| PDB annotation | TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DIA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULATIONINA) YING-YANG I; TRANSCRIPTION INITIATION, INITIATIOR ELEMENT, YYI, ZINC 2 FINGER PROTEIN, UNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | COMPLEX (TRANSCRIPTION REGULATIONINA) YING-YANG I; TRANSCREPTON INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX RECOGNITION, 3 COMPLEX | COMPLEX (TRANSCRIPTION REGULATIONINA) YING-YANG I; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATIONDNA) | ZINC FINGER DNA BINDING DOMAIN DNA BINDING MOTIF, ZINC FINGER DNA BINDING DOMAIN | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) |
| Coumpound | INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | YYI; CHAIN: C, ADENO- ASSOCIATED VIRUS PS INITATOR ELEMENT DNA; CHAIN: A, B; | YY I; CHAIN: C; ADENO- ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA; CHAIN: A, B; | SWIS; CHAIN: NULL; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; |
| SeqFold score | | | 86.51 | | | | | |
| PMF | | 0.98 | | - | 0.72 | 96'0 | _ | - |
| Verify score | | 0.43 | | 90:0- | 0.15 | -0.04 | -0.21 | -0.1 |
| PSI- BLAST | | 5.40E-51 | 5.40E-51 | 3.20E-34 | 0.00016 | 3.20E-31 | 3.60E-52 | 5.40E-63 |
| End AA | | 640 | 641 | 640 | 642 | 276 | 307 | 363 |
| Start | | 529 | 531 | . 239 | 615 | 140 | 170 | 197 |
| Chain | | υ | ပ | ပ | | ∀ | ∢ | ∢ . |
| 808 CI | | lubd | lubd | Inpq | pjzt | 2gli | 2gli | 2gli |
| S a S | | 098 | 098 | 098 | 098 | 98 | 098 | 098 |

| PDB annotation | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINDNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEINIDNA) | COMPLEX (DNA-BINDING PROTEINDNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTFINDNA) | COMPLEX (DNA-BINDING |
|------------------|--|--|--|--|--|--|---|--|---|--|---------------------------|
| Coumpound | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D: | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; |
| SeqFold score | | | | | | | | | | | 91.33 |
| PMF | _ | 86.0 | 0.99 | 0.19 | 6:0 | 0.49 | 61.0 | 0.99 | _ | _ | |
| Verify score | 0.06 | 0.13 | 0.25 | -0.4 | 0.03 | -0.21 | -0.07 | -0.02 | 0.27 | 0.53 | |
| PSI- BLAST | 3.60E-64 | 1.60E-33 | 1.80E-64 | 3.60E-57 | 1.30E-34 | 1.60E-32 | 5.40E-60 | 1.30E-30 | 1.40E-35 | 3.60E-64 | 3.60E-64 |
| End | 391 | 360 | 447 | 558 | 444 | 527 | 614 | 286 | 119 | 640 | 642 |
| Start | 224 | 722 | 280 | 308 | 316 | 400 | 421 | 456 | 484 | 503 | 503 |
| Chain ID | ٧ | ¥ | V | ٧ | ٧ | ٧ | V | A | ٧ | ¥ | ¥ |
| EDB ID | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli | 2gli |
| SEQ D NO: | 098 | 098 | 098 | 098 | 098 | 098 | 098 | 098 | 098 | 098 | 980 |

| | | | | _ | | | | | | |
|------------------|--|--|--|---|--|---|---|---|---|--|
| PDB annotation | PROTEIN/DNA) FIVE-FINGER GLJ; GLJ, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA) | HYDROL YTC ENZYME DLH; DIENELACTONE HYDROLASE, AROMATIC HYDROCARBON CATABOLISM, 2 SERNE ESTERASE, CARBOXYMETHYLENEBUTENOLIDA SE, 3 HYDROLYTIC ENZYME | | COMPLEX OF TWO ELONGATION FACTORS EFT-U, EFT-3; ELONGATION FACTOR, NUCLEOTIDE EXCHANGE, GTP-BINDING, 2 COMPLEX OF TWO ELONGATION FACTORS | COMPLEX (TWO ELONGATION FACTORS) ELONGATION FACTOR FOR TRANSPER, HEAT UNSTABLE, ELONGATION FACTOR FOR TRANSPER, HEAT STABLE, ELONGATION FACTOR, COMPLEX ELONGATION FACTOR, COMPLEX (TWO ELONGATION FACTOR) | DNA-BINDING HMGA DNA-BINDING HMG-BOX DOMAIN A OF RAT HMGI; IAAB 8 HMG-BOX IAAB 20 | DNA-BINDING HMGA DNA-BINDING HMG-BOX DOMAIN A OF RAT HMGI; JAAB 8 HMG-BOX JAAB 20 | DNA-BINDING HMGA DNA-BINDING HMG-BOX DOMAIN A OF RAT HMG1; JAAB 8 HMG-BOX 1AAB 20 | DNA BINDING PROTEIN HMG BOX, DNA BENDING, DNA RECOGNITION, CHROMATIN, NMR, DNA 2 BINDING |
| Coumpound | CHAIN: A; DNA; CHAIN: C, D; | ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D; | DIENELACTONE HYDROLASE; CHAIN: NULL; | | ELONGATION FACTOR TU; CHAIN: A, B, E, F; ELONGATION FACTOR TS; CHAIN: C, D, G, H; | ELONGATION FACTOR TU; CHAIN: A, C; ELONGATION FACTOR TS; CHAIN: B, D; | HIGH MOBILITY GROUP PROTEIN; 1AAB 5 CHAIN: NULL; 1AAB 6 | HIGH MOBILITY GROUP PROTEIN; 1AAB 5 CHAIN: NULL: 1AAB 6 | HIGH MOBILITY GROUP PROTEIN; 1AAB 5 CHAIN: NULL: 1AAB 6 | NON HISTONE PROTEIN 6 A; CHAIN: A; |
| SeqFold score | | | | | | | | | | |
| PMF score | | 0.46 | 96.0 | | 99.0 | 0.75 | 68.0 | - | 0.33 | 96.0 |
| Verify score | | -0.16 | 0.02 | | 0.02 | -0.56 | -0.09 | 89:0 | 0.41 | -0.12 |
| PSI- BLAST | | 1.40E-36 | 0.00013 | | 0.00018 | 0.00018 | 9.00E-18 | 5.40E-16 | 1.80E-06 | 1.80E-16 |
| End | | 279 | 338 | | 2676 | 2673 | 185 | 433 | 290 | 180 |
| Start AA | | 95 | 255 | | 2646 | 2646 | 106 | 363 | 528 | 112 |
| Chain D | | ¥ | | | ပ | æ | | | | ∢ |
| PDB CD | | 2gli | 1din | | laip | lefu | laab | laab | laab | 1cg7 |
| SEQ B B S | | 980 | 862 | | 864 | 864 | 865 | 865 | 865 | \$98 |

| | | r | | | | | | | |
|------------------|---------|---|---|---|---|--|---|--|--|
| PDB annotation | PROTEIN | DNA BINDING PROTEIN HMG BOX, DNA BENDING, DNA RECOGNITION, CHROMATIN, NMR, DNA 2 BINDING PROTEIN | DNA BINDING PROTEIN HMG BOX, DNA BENDING, DNA RECOGNITION, CHROMATIN, NMR, DNA 2 BINDING PROTEIN | DNA BINDING PROTEIN HMG BOX, DNA BENDING, DNA RECOGNITION, CHROMATIN, NMR, DNA 2 BINDING PROTEIN | DNA BINDING PROTEIN HMG BOX, DNA BENDING, DNA RECOGNITION, CHROMATIN, NMR, DNA 2 BINDING PROTEIN | GENE REGULATION/DNA HIMG-1, AMPHOTERIN, HERSARIN-BINDING PROTEIN P30; HIGH-MOBILLTY GROUP DOMAN, BENT DNA, PROTEIN-DNGUE-DNA, 2 COMPLEX, GENE REGULATION/DNA | GENE REGULATION/DNA HIMG-1, AMPHOTERIN, HERSARIN-BINDING PROTEIN PJO: HIGH-MOBILLITY GROUP DOMAIN, BENT DNA, PROTEIN-DNGUG-DABA, Z COMPLEX, GENE REGULATION/DNA | GENE REGULATION/DNA HMG-1, AMPHOTERN, HERSARD-BINDING PROTEIN PRO HERSARD-BINDING PROTEIN PRO HIGH-MOBILITY GROUP DOMAIN, BENT DNA, PROTEIN-DNGUE-DNA-2 COMPLEX, GENE REGULATION/DNA | GENE REGULATION/DNA HMG-1, AMPHOTERNI, HERSARID-BINDING PROTEIN P30: HIGH-WOBILLTY GROUP DOMAIN, BENT DNA, PROTEIN-DNGLG-DNA, Z COMPLEX, GENE REGULATION/DNA |
| Coumpound | | NON HISTONE PROTEIN 6 A; CHAIN: A; | HIGH MOBILITY GROUP I PROTEIN; CHAIN: A; DNA (5'- DY'CP*CP*(TP*(DO) CHAIN: B; DNA (5'- CHAIN: C; | HIGH MOBILITY GROUP I PROTEIN; CHAIN: A; DNA (5:- D(*CP*CP*(DD) CHAIN: B; DNA (5:- CHAIN: C; | HIGH MOBILITY GROUP I PROTEIN; CHAIN: A; DNA (5- D(*CP*CP*(TDO) CHAIN: B; DNA (5- CHAIN: C; | HIGH MOBILITY GROUP I PROTEIN; CHAIN: A; DNA (5'- D(*CP*CP*(IDO) CHAIN: B; DNA (5'- CHAIN: C; |
| SeqFold score | | | | | | | | | |
| PMF | | 0.83 | _ | 0.42 | 0.24 | 0.92 | 0.71 | 0.99 | 0.11 |
| Verify score | | 0.3 | 0.45 | -0.4 | 0.28 | -0.29 | 0.02 | 0.4 | 0.03 |
| PSI- BLAST | | 3.60E-07 | 5.40E-16 | 7.20E-06 | 1.80E-06 | 5.40E-14 | 3.60E-07 | 3.60E-15 | 7.20E-05 |
| End | | 320 | 433 | 516 | 109 | 171 | 320 | 433 | 510 |
| Start AA | | 262 | 369 | 476 | 532 | 112 | 262 | 369 | 476 |
| Chain ID | | Ą | ¥ | A | Y | ¥ | ¥ | V | ¥ |
| PDB ID | | lcg7 | lcg7 | lcg7 | lcg7 | lokt | lckt | 1ckt | r r r |
| SEQ No de | | 865 | 865 | 865 | 865 | 865 | 865 | 865 | 865 |

| PDB annotation | GENE REGULATION/DNA HMG-1, AMPHOTERN, HERSARIN-BINDING PROTEIN 790; HIGH-MOBILLITY GROUP DOMAIN, BENT DNA, PROTEIN-DRUG-DNA Z COMPLEX, GENE REGULATION/DNA | STRUCTURAL PROTEIN TWO REPEATS OF SPECTRIN, ALPHA HELICAL LINKER REGION, 2 2 HADDEM 3-HELIX COLED-COILS, STRUCTURAL PROTEIN | | | | COMPLEX (DNA-BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) | |
|-----------------|--|---|--|--|--|--|--|---|
| Coumpound | HIGH MOBILITY GROUP 1 PROTEIN, CHAIN: A; DNA (5'- D("CP"CP"(IDO) CHAIN: B; DNA (5'- CHAIN: C; | ALPHA SPECTRIN; CHAIN: A, B, C; | DNA-BNDING HIGH MOBILITY GROUP PROTEIN FRAGMENT-B (HMGB) (DNA-BINDING 1 HME 3 HMG-BOX DONAIN B OF RAT HMG1) (NMR, 1 STRUCTIRE) 1 HME 4 | DNA-BINDING HIGH MOBILITY GROUP PROTEIN FRAGMENT-B (HMGB) (DNA-BINDING 1 HME 3 HMG-BOX DONAIN B OF RAT HMG! (VMR, 1 STRUCTURE) 1 HME 4 | DNA-BINDING HIGH MOBILITY GROUP PROTEIN FRAGMENT-B (HMGB) (DNA-BINDING I HME 3 HMG-BOX DOMAIN B OF RAT HMG! (NMR, I STRUCTURE) I HME 4 | HUMAN SRY; IHRY 6 CHAIN: A; IHRY 7 DNA; IHRY 9 CHAIN: B: IHRY 10 | HUMAN SRY; IHRY 6 CHAIN: A; IHRY 7 DNA; IHRY 9 CHAIN: B; IHRY 10 | DNA-BINDING HIGH MOBILITY GROUP PROTEIN 1 (HMGI) BOX 2, |
| SeqFold | | | | | | | | |
| PMF score | 0.01 | 0 | 0.57 | 0.43 | - | 0.39 | 0.78 | 0.21 |
| Verify score | -0.01 | -0.16 | 0 | -0.19 | 0.04 | -0.52 | 0.19 | 0.44 |
| PSI- BLAST | 1.40E-05 | 7.20E-08 | 3.60E-14 | 0.00036 | 3.60E-13 | 9.00E-15 | 1.80E-16 | 9.00E-12 |
| End | 290 | 285 | 160 | 303 | 418 | 081 | 433 | 160 |
| Start | 530 | 382 | 107 | 257 | 369 | 011 | 368 | 112 |
| Chain Th | < | ∢ | | | | ¥ | A | |
| PDB ID | lckt | lcun | Ihm e | e e | e e | lhry | Ihry | Thsm . |
| ğ a ÿ | 865 | 865 | \$98 | 88 | 865 | 865 | 865 | 865 |

| PDB annotation | | | | GENE REGULATION/DNA HMG-D; PROTEIN-DNA COMPLEX, HMG DOMAIN, NON-SEQUENCE SPECIFIC 2 CHROMOSOMAL PROTEIN HMG-D | GENE REGULATION/DNA HMG-D; PROTEIN-DNA COMPLEX, HMG DOMAIN, NON-SEQUENCE SPECIFIC 2 CHROMOSOMAL PROTEIN HMG-D | GENE REGULATIONDNA LEF-I HMG; LEFI, HMG, TCR-A, TRANSCRIPTION PACTOR, DNA BINDING, DNA 2 BENDING, COMPLEX (HMG DOMANIDNA), GENE REGULATIONDNA, GENE | GENE REGULATION/DNA LEF-1 HMG; LEFI, HMG, TCR-A, TRANSCRIPTION FACTOR, DNA, BINDING, DNA 2 BENDING, COMPLEX (HMG DOMANDINA), GENE REGILLATION/DNA | GENE REGULATION/DNA LEF-I HMG; |
|------------------|---|---|---|--|---|--|--|--------------------------------|
| Coumpound | COMPLEXED WITH 1HSM 3 MERCAPTOETHANOL (NMR, MINIMIZED AVERAGE STRUCTURE) 1HSM 4 | DNA-BINDING HIGH MOBILITY GROUP PROTEIN 1 (FIMCI) BOX 2, COMPLEXED WITH 1HSM 3 MERCATPOETHANOL (NMR, MINIMIZED AVERAGE STRUCTURE) HSM 4 | DNA-BINDING HIGH MOBILITY GROUP PROTEIN I (RMG1) BOX 2, COMPLEXED WITH 1HSM 3 MERCATDETHANOL (NMR, MINIMIZED AVERAGE STRUCTURD 1HSM 4 | DNA (5°- D(*GP*CP*GP*AP*TP*AP*TP *CP*GP*CJ-3'), CHAIN: C, D; HIGH MOBILITY GROUP PROTEIN D, CHAIN: A, B; | DNA (5'- D(*GP*CP:QP*AP*AP*TP *CP*GP*CJ-3'), CHAIN: C, D; HIGH MOBILITY GROUP PROTEIN D; CHAIN: A, B; | LYMPHOID ENHANGER- BINDING FACTOR; CHAIN: A; DNA (5'-CHAIN: B; DNA (5'-CHAIN: C; | LYMPHOID ENHANCER- BINDING FACTOR; CHAIN: A; DNA (5'- CHAIN: B; DNA (5'- CHAIN: C; | LYMPHOID ENHANCER- |
| SeqFold score | | | | | | | | |
| PMF | | 0.37 | _ | 0.01 | 0.78 | 0.36 | 0.58 | - |
| Verify score | | 0.02 | 9:0 | -0.69 | 0.18 | -0.23 | 0.11 | 0.76 |
| PSI- BLAST | | 0.00036 | 5.40E-13 | 1.10E-10 | 5.40E-12 | 1.80E-14 | 3.60E-07 | 1.10E-14 |
| End | | 303 | 418 | 153 | 411 | 180 | 320 | 433 |
| Start AA | | 262 | 369 | 112 | 367 | 1113 | 262 | 371 |
| Chain ID | | | | ∢ | ¥ | ¥ | « | A |
| PDB ID | | Ihsm | lhsm | Iqrv | 1qrv | 21cf | 2lef | 2lef |
| SEQ B OS | | 865 | 865 | 865 | 865 | 865 | 865 | 865 |

| PDB annotation | LEFI, HMG, TCR-A, TRANSCRIPTION FACTOR, DNA BINDING, DNA 2 BENDING, COMPLEX (HMG DOMAINDINA), GENE REGULATIONDNA | GENE REGULATIONDNA LEF-1 HMG, LEFI, HMG, TCR-4, TRANSCRIPTION PACTOR, DNA BINDING, DNA 2 BENDING, COMPLEX (HMG DOMANDINA), GENE REGULATIONDNA, | COMPLEX (TRANSDUCERTRANSDUCTION) GT (TRANSDUCERTRANSDUCTION) GT BETT-A-GAMMA, MEKA, PP3; PHOSDUCIN, TRANSDUCIN, BETT-A- GAMMA, SIGNAL TRANSDUCTION, 2 FEGULATION, PHOSPHORYLATION, OF PROTINS, THIOREDOXIN, 3 VISION, MEKA, COMPLEX (TRANSDUCERTRANSDUCTION) | ENDOCYTOSIS/EXOCYTOSIS SYNAPTOTAGMIN ASSOCIATED 35 KDA PROTEIN, P35A, THREE HELIX BUNDLE | CONTRACTILE PROTEIN TRIPLE- HELIX COILED COIL, CONTRACTILE PROTEIN | ISOMERASE ISOMERASE, MUTASE, INTRAMOLECULAR TRANSFERASE | ISOMERASE ISOMERASE, MUTASE, INTRAMOLECULAR TRANSFERASE | TRANSCRIPTION REGULATION SIGMATO; RNA POLYMERASE SIGMA FACTOR, TRANSCRIPTION REGULATION | TRANSFERASE GLYCOSYLTRANSFERASE |
|-----------------|--|---|--|--|--|--|--|---|--|
| Coumpound | BINDING FACTOR, CHAIN: A; DNA (5'-CHAIN: B; DNA (5'-CHAIN: C; | LYMPHOID ENHANCER. BINDING FACTOR; CHAIN: A; DNA (\$'-CHAIN: B; DNA (\$'-CHAIN: C; | TRANSDUCIN; CHAIN: P, PHOSDUCIN; CHAIN: P, | SYNTAXIN-IA; CHAIN: A, B, C; | HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A; | METHYLMALONYL-COA MUTASE; CHAIN: A, B, C, D; | METHYLMALONYL-COA MUTASE; CHAIN: A, B, C, D; | RNA POLYMERASE PRIMARY SIGMA FACTOR; CHAIN: NULL; | SPORE COAT POLYSACCHARIDE BIOSYNTHESIS PROTEIN CHAIN: A; |
| SeqFold | | | | | | | | | |
| PMF | | 99.0 | -0.19 | -0.2 | -0.19 | -0.2 | -0.19 | -0.19 | 0.22 |
| Verify score | | 0.28 | 0.78 | 0.53 | 0.58 | 0.36 | 0.64 | 0.09 | 0.06 |
| PSI- BLAST | | 3.60E-06 | 3.60E-12 | 1.80E-09 | 5.40E-09 | 3.60E-12 | 1.80E-10 | 1.80E-08 | 0.0018 |
| End | | 290 | 709 | 465 | 467 | 464 | 482 | 463 | 302 |
| Start AA | | 332 | 639 | 396 | 396 | 390 | 396 | 386 | 24 |
| Chain D | | ∢ | p. | V | ∢ . | ∢ ' | V | | ∢ |
| 808 CI | | 2lef | 2trc | lez3 | lquu | Ireq | lreq | 1sig | lqgq |
| SEQ No. B | | 865 | 865 | 998 | 866 | 866 | 866 | 998 | 871 |

| PDB annotation | RNA-BINDING PROTEINRNA TRA PRE-MRNA; SPLICING REGULATION, RNP DOMAIN, RNA COMPLEX | GENE REGULATIONRNA POLY(A) BINDING PROTEIN I, PABP I, RRM, PROTEIN-RNA COMPLEX, GENE REGULATIONRNA | GENE REGULATIONRNA POLY(A) BINDING ROTGEN I, PABP I, RRM, PROTEIN-RNA COMPLEX, GENE REGULATIONRNA | GENE REGULATIONRNA POLY(A) BINDING PROTEIN I, PABP 1; RNA, PROTEIN-RNA COMPLEX, GENE REGULATIONRNA | GENE REGULATIONRNA POLY(A) BINDING ROTGEN I, PABP I, RRM, PROTEIN-RNA COMPLEX, GENE REGULATIONRNA | RNA BINDING PROTEIN RNA- BINDING DOMAIN | NUCLEAR PROTEIN HETROGOBBOUS NUCLEAR RIBONUCLEOPROTEIN AI, NUCLEAR PROTEIN, HNRNP, RBD, RRM, RNP, RNA BINDING, 2 RIBONUCLEOPROTEIN RIBONUCLEOPROTEIN | |
|-----------------|---|--|---|--|--|--|--|--|
| Coumpound | SXL-LETHAL PROTEIN; CHAIN, A. B. RNA (5'- R(P*GP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP | POLYDENYLATE BINDING PROTEIN I; CHAIN: A, B, C, D, E, F, G, H; RNA (5'- R(*AP*AP*AP*AP*AP*AP*AP*AP AAP*AP*AP*AP; CHAIN: AAP*AP*AP*AP; CHAIN: | POLYDENYLATE BINDING PROTEIN I; CHAIN: A, B, C, D, E, F, G, H; RNA (5'- R(*AP*AP*AP*AP*AP*AP*AP AAP*AP*AP*AP*AP*AP*AP*AP M, N, O, P, Q, R, S, T; | POLYDENYLATE BINDING PROTEIN I; CHAIN: A, B, C, D, E, F, G, H: RNA (5'- R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP* | POLYDENYLATE BINDING PROTEIN I; CHAIN: A, B, C; D, E, F, G, H; RNA (5'- R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP* | HU ANTIGEN C; CHAIN: A; | HNRNP A1; CHAIN: NULL; | RNA-BINDING PROTEIN SEX-LETHAL PROTEIN (C- TERMINUS, OR SECOND |
| SeqFold | | | | | | | | |
| PMF | - | 0.92 | - | - | _ | <u>.</u> | - | 0.92 |
| Verify score | 0.52 | 0.52 | 66'0 | 0.92 | 26.0 | 0.83 | 0.48 | 0.56 |
| PSI- BLAST | 1.40E-21 | 6.40E-24 | 1.60E-20 | 1.60E-20 | 1.60E-20 | 1.10E-21 | 3.20E-22 | 1.40E-21 |
| End AA | 104 | 110 | 106 | 901 | 106 | 106 | 124 | 109 |
| Start | 9 | 9 | 27 | 7.7 | 7.7 | . 52 | 21 | 24 |
| Chain El | ¥ | ¥ | ш | tr. | н | ٧ | | |
| PDB ED | 1b7f | lovj | lcvj | lcvj | lcvj | 148z | lhal | lsxl |
| SEQ NO: | 872 | 872 | 872 | 872 | 872 | 872 | 872 | 872 |

| PDB annotation | | COMPLEX RIBONUCLEOPROTEIN/DNA) HRINP AL DPI, COMPLEX RIBONUCLEOPROTEIN/DNA), HETEROGENEOUS NUCLEAR 2 KIBONUCLEOPROTEIN A1 | RNA BINDING DOMAIN RNA BINDING DOMAIN, RBD, RNA RECONTITION MOTIF, RRAY, 2 SPLCING INHIBITOR, TRANSLATIONAL INHIBITOR, SEX 3 DETERMINATION, X CRROMOSOME DOSAGE COMPENSATION | CALCIUM/PHOSPHOLIPID BINDING RROTEIN PHI, CALPACITIN LIGHT CRANK, SI NG FAMILY, EF-HAND PROTEIN, LIGAND OF ANNEXIN II, 2 CALCIUM/PHOSPHOLIPID BINDING RROTEIN | CALCIUM-BINDING CNTNC; CALCIUM-BINDING, REGULATION, TROPONIN C, CARDIAC MUSCLE 2 CONTRACTION | CALCTUM BINDING CALCTUM BINDING | METAL BINDING PROTEIN CAVP, EF- HAND FAMILY, CALCIUM BINDING PROTEIN, NMR | | |
|------------------|--|--|---|--|---|--|---|---|--|
| | | COMPLEX (RIBONUC A1, UP1; C (RIBONUC HETEROG RIBONUC | RNA I DOM/ MOTE TRAN DETE DOSA | CALCIUM PROTEIN CHAIN; SI PROTEIN, CALCIUM PROTEIN | SALC SALC SON SON SON SON SON SON SON SON SON SON | CALCTUM | HANE PROT | | |
| Coumpound | RNA-BINDING DOMAIN 1SXL3 (RBD-2), RESIDUES 199 - 294 PLUS N-TERMINAL MET) 1SXL 4 (NMR, 17 STRUCTURES) 1SXL 5 | HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN A1; CHAIN: A; 12-NUCLEOTIDE SINGLE-STRANDED TELOMETRIC DNA; CHAIN: B: | SEX-LETHAL; CHAIN: A, B, C; | S100A10; CHAIN: A, B; | CARDIAC N-TROPONIN C; CHAIN: NULL; | CALCIUM-BINDING PROTEIN; CHAIN: NULL; | CALCIUM VECTOR PROTEIN; CHAIN: A; | CALCIUM-BINDING PROTEIN CALBINDIN D9K (INTACT FORM) (NMR, 13 STRUCTURES) 1CB1 3 | CALCIUM-BINDING PROTEIN CALMODULIN (VERTEBRATE) ICLL 3 |
| SeqFold score | | | j | , | | | | | |
| PMF | | 0.99 | 0.99 | 1 | 0.29 | 0.15 | 0.16 | _ | 0.16 |
| Verify score | | 0.68 | 0.58 | 0.66 | -0.25 | -0.05 | -0.22 | 0.35 | -0.14 |
| PSI- BLAST | | 1.30E-22 | 1.60E-20 | 7.20E-18 | 9.00E-07 | 5.40E-07 | 7.20E-07 | 9.00E-22 | 3.60E-07 |
| End | | 124 | 104 | 93 | 11 | 82 | 78 | 83 | 35 |
| Start AA | | 61 | 9 | | 21 | 22 | 22 | ∞ · | = |
| Chain ID | | ∢ | ¥ | ∢ | | | Ą | | |
| EDB EDB | | 2up1 | 3sxl | 1а4р | lap4 | 1bu3 | lc7w | 1001 | ıcıı |
| SeQ No B | | 872 | 872 | 873 | 873 | 873 | 873 | 873 | 873 |

| | | | | _ | | _ | | | | | | _ |
|-----------------|---|--|--|---|--|---|---|---|--|---|--|---|
| PDB annotation | METAL BINDING PROTEIN YEAST FREQUENIN EF-HAND, CALCIUM | METAL TRANSPORT MRPB, S100AB, CALGRANULIN A CALCINA-BINDING PROTEIN, CRYSTAL STRUCTURE, MAD, MIGRATION 2 INHIBITORY FACTOR, RELATED PROTEIN 8, S100 PROTEIN | COMPLEX (LIGAND/ANNEXIN) CALOZZARNI, SIOP PAMILY, EF. HAND PROTEIN, COMPLEX (LIGAND/ANNEXIN), 2 LIGAND OF ANNEXINI, ANNEXINI, ROTEIN PROTEIN | | HYDROLASE CEREBROSIDE-3- ULFATE-SULFATASE; CEREBROSIDE-3-SULFATE HYDROLYSIS, LYSOSOMAL ENZYME, 1 HYDROLASE | | LYASE DELTA3,5,DELTA2,4- DIENOYL-COENZYME A ISOMERASE, LYASE, DIENOYL-COA ISOMERASE | LYASE DELTA3,5,DELTA2,4- DIENOYL-COENZYME A ISOMERASE, LYASE, DIENOYL-COA ISOMERASE | LYASE METHYLMALONYL COA, DECARBOXYLASE | LYASE DEHALOGENASE; LYASE | LYASE CROTONASE, ENOYL-COA HYDRATASE I: LYASE, HYDRATASE, B-OXIDATION, FATTY ACID DEGRADATION, COA, 2 LIGAND BINDING | |
| Coumpound | CALCIUM-BINDING PROTEIN NCS-1; CHAIN: A; | MIGRATION INHIBITORY FACTOR-RELATED PROTEIN 8; CHAIN: A, B; | S100C PROTEIN; CHAIN: A; Annexin I; Chain: D; | | ARYLSULFATASE A; CHAIN: NULL; | | DIENOYL-COA ISOMERASE; CHAIN: A, B, C; | DIENOYL-COA ISOMERASE; CHAIN: A, B, C; | METHYLMALONYL COA DECARBOXYLASE; CHAIN: A, B, C; | 4-CHLOROBENZOYL COENZYME A DEHALOGENASE; CHAIN: A, B, C; | 2-ENOYL-COA HYDRATASE; CHAIN: A. B, C, D. E, F: | |
| SeqFold | | | | | | | | | | | | |
| PMF | 10.0 | 0.81 | | | 0.46 | | 0.17 | 0.35 | 0.01 | -0.11 | 0.13 | |
| Verify score | -0.07 | 0.15 | 0.38 | | 0.29 | | -0.17 | -0.02 | -0.23 | 0.3 | -0.11 | |
| PSI- BLAST | 9.00E-08 | 1.80E-17 | 1.80E-18 | | 9.60E-65 | | 1.80E-14 | 3.20E-22 | 1.60E-18 | 4.80E-21 | 3.20E-24 | |
| End A.A. | 81 | 88 | 92 | | 330 | | 121 | 144 | 145 | 144 | 144 | |
| Start AA | = | - | œ | | 39 | | 48 | \$\$ | 45 | 47 | 47 | |
| Chain ID | ٧ | ∢ | ∢ | | | | Ą | ٧ | ٧ | ¥ | 4 | |
| PDB ID | Ifpw | 1mr8 | 1qis | | lauk | | 1dci | Idei | lef8 | lnzy | 2dub | |
| SEQ NO: D | 873 | 873 | 873 | | 874 | | 875 | 875 | 875 | 875 | 878 | |

| | | | | _ | , | | | | | _ | | | _ | | | _ | | _ | | _ | | | | | | | |
|-----------------|---|---|---|---|---|------|--------------------------|-------------------------------|------------------------------|----------------------------|----------------------------|---|----------------------------|--------------------------|--|-------------------------------|---------------------------------|-------------------------------|----------------|-------------------------------|---------------------------------|-------------------------------|-----------------------------------|-------------------|------------------------|--|--|
| PDB annotation | UBIQUITIN CONTUGATION UBC2; UBIQUITIN CONTUGATION, UBIQUITIN-CONTUGATING ENZYME | UBIQUITIN CONJUGATION UBC2; UBIQUITIN CONJUGATION, UBIQUITIN-CONJUGATING ENZYME | LIGASE UBIQUITIN, UBIQUITIN- CONJUGATING ENZYME, YEAST | LIGASE UBIQUITIN, UBIQUITIN- CONJUGATING ENZYME, YEAST | LIGASE UBIQUITIN, UBIQUITIN- CONJUGATING ENZYME, YEAST | | SIGNALLING COMPLEX RACI; | GTPASE NADPH OXIDASE PROTEIN- | PROTEIN 2 COMPLEX, TPR MOTIF | | CHAPERONE HOP, TPR-DOMAIN, | PEPTIDE-COMPLEX, HELICAL REPEAT, HSP90, 2 PROTEIN BINDING | CHAPERONE HOP, TPR-DOMAIN, | PEPTIDE-COMPLEX, HELICAL | REPEAT, HSC70, 2 HSP70, PROTEIN BINDING | SIGNALING PROTEIN PEROXISMORE | RECEPTOR 1, PTS1-BP, PEROXIN-5, | FISH PROTEIN-PEPTIDE COMPLEX, | HELICAL REPEAT | SIGNALING PROTEIN PEROXISMORE | RECEPTOR 1, PTS1-BP, PEROXIN-5, | PISI PROTEIN-PEPTIDE COMPLEX, | HELIKALKICOPEPIIDE KEPEAI, IPK, 2 | ווייים ואין וייין | OXIDOREDUCTASE | OXIDOREDUCIASE, IROPANE ALKALOID RIOSVNTHESIS | REDUCTION OF 2 TROPINONE TO TROPINE, SHORT-CHAIN |
| Coumpound | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, C; | UBIQUITIN-CONJUGATING ENZYME RAD6, CHAIN: A, B, C; | UBIQUITIN CONJUGATING ENZYME; CHAIN: A; | UBIQUITIN CONJUGATING ENZYME; CHAIN: A; | UBIQUITIN CONJUGATING ENZYME; CHAIN: A; | | RAS-RELATED C3 | SUBSTRATE 1: CHAIN: A: | NEUTROPHIL CYTOSOL | FACTOR 2 (NCF-2) CHAIN: B; | TPR2A-DOMAIN OF HOP; | CHAIN: A; HSP90-PEPTIDE MEEVD: CHAIN: B: | TPR1-DOMAIN OF HOP; | CHAIN: A, B; HSC70- | PEPTIDE; CHAIN: C, D; | PEROXISOMAL TARGETING | SIGNAL I RECEPTOR; | CONTABING PERTING | CHAIN: C, D; | PEROXISOMAL TARGETING | SIGNAL I RECEPTOR; | CHAIN: A, B; PTS1- | CHADI: C D. | CIOIL: C, E, | TROPINONE REDUCTASE-I; | CHAIN: A, B; | |
| SeqFold | 139.32 | | 226.34 | | | | | | | | | | | | | | | | | | | | | | | | |
| PMF | | 1 | | _ | - | | -0.14 41.0 | | | | -0.15 | | -0.19 | | | -0.18 | | | | -0.18 | | | | | ÷ | | |
| Verify score | | 0.84 | | 0.91 | 0.71 | | 0.15 | | | | 0.31 | | 0.02 | | | 0.04 | | | | 0.01 | | | | | 0.35 | | |
| PSI- BLAST | 3.60E-63 | 3.60E-63 | 9.00E-63 | 9.00E-63 | 4.80E-62 | | 3.20E-09 | | | | 1.60E-18 | | 8.00E-09 | | | 4.80E-14 | | | | 1.40E-23 | | | | | 6.40E-29 | | |
| End | 151 | 146 | 147 | 147 | 146 | , | 137 | | | | 112 | | 153 | | | 157 | | | | 241 | | | | | 141 | | |
| Start AA | - | 2 | _ | 2 | 3 | | 12 | | | | 7 | | 22 | | | _ | | | | 12 | | | | | 33 | | |
| Chain ID | A | ¥ | ¥ | A | A | 1 | m | | | | ∢ | | ٧ | | | Ą | | | | ٧ | | | | | ٧ | | |
| EDB CI | layz | layz | ldcd | lqcq | Iqeq | | 1.00 | 3 | | | 洁 | | lelw | | | 1fch | | | | lfch | | | | П | laci | | |
| SEQ NO ED | 877 | 877 | 877 | 212 | 877 | 0.00 | 878 | | | | 878 | | 878 | | | 878 | | | | 878 | | | | | 881 | | |

| | _ | | | | | | | | | |
|------------------|---------------|--|---|--|--|---|--|---|--|-------------------------|
| PDB annotation | DEHYDROGENASE | OXIDOREDUCTASE ROYALOID BIOSYNTHESIS, REDUCTION OF 2 TROPINONE TO TROPINE, SHORT-CHAIN DEHYDROGENASE | OXIDOREDUCTASE OXIDOREDUCTASE, OXIDOREDUCTASE, ALCOHOL 2 DEHYDROGENASE, BROSOHILA LEBANONENSIS, SHORT-CHAIN B. DEHYDROGENASE/REDUCTASES, TENNARY COMPLEX, NAD-3- PENTANONE A ADDUCT | OXIDOREDUCTASE NAD-DEPENDENT OXIDOREDUCTASE, SHORT-CHAIN ALCOHOL 2 DEHYDROGENASE, PCB DEGRADATION | OXIDOREDUCTASE SHORT-CHAIN DEHYDROGENASE, OXIDOREDUCTASE | OXIDOREDUCTASE SHORT-CHAÎN DEHYDROGENASEREDUCTASE, BILE ACID CATABOLISM | | OXIDOREDUCTASE SEPIAPTERIN REDUCTASE, TETRAHYDROBIOPTERIN, OXIDOREDUCTASE | OXIDOREDUCTASE NAPHTHOL REDUCTASE; OXIDOREDUCTASE | OXIDOREDUCTASE |
| Coumpound | | TROPINONE REDUCTASE-I; CHAIN: A, B; | ALCHOJ DEHYDROGENASE; CHAIN: A, B; | CIS-BIPHENYL-2,3- DIHYDRODIOL-2,3- DEHYDROGENASE; CHAIN: NULL; | CARBONYL REDUCTASE; CHAIN: A, B, C, D; | 7 ALPHA- HYDROXYSTEROID DEHYDROGENASE; CHAIN: A, B; | OXIDOREDUCTASE 3. ALPHA, 20BETA. HYDROXYSTEROID DEHYDROGENASE (E.C. I.1.1.5) I IHDC 3 COMPLEXED WITH CARBENOXOLONE I HDC 4 | SEPIAPTERIN REDUCTASE; CHAIN: NULL; | TRIHYDROXYNAPHTHALEN E REDUCTASE; CHAIN: A, B; | TROPINONE REDUCTASE-II; |
| SeqFold score | | | | | | | | | | |
| PMF | | - | 6:0 | 0.93 | 0.98 | _ | 0.99 | 6.0 | | 0.99 |
| Verify | | 0.36 | 0.14 | 0.32 | 0.1 | 89:0 | 0.34 | 0.47 | 0.38 | 0.49 |
| PSI- BLAST | | 6.40E-29 | 1.40E-21 | 1.60E-24 | 4.80E-21 | 1.60E-34 | 1.10E-29 | 1.80E-20 | 4.80E-33 | 6.40E-29 |
| End AA | | 147 | 129 | 147 | 148 | 147 | 148 | 129 | 147 | 147 |
| Start AA | | 33 | 38 | 36 | 36 | 31 | 35 | 38 | 23 | 31 |
| Chain | | æ | ⋖ | | ¥ | V | ∢ | | ∢ | Ą |
| 80 a | - | lael | 1616 | 1bd | lcyd | Ifmc | Ihdc | loaa | 1ybv | 2ac2 |
| S B S | | 8881 | 888 | 881 | 881 | 1881 | 188 | 881 | 881 | 881 |

| | | _ | | | | | | | | | | | | | |
|------------------|---|---|---|---|---|-------------------------------|---|------------------------------|--|--|--|---|--|---|-----------------------|
| PDB annotation | OXIDOREDUCTASE, TROPANE ALKALOID BIOSYNTHESIS, REDUCTION OF 2 TROPINONE TO PSEUDOTROPINE, SHORT-CHAIN DEHYDROGENASE | | UBIQUITIN CONIUGATION UBC2; UBIQUITIN CONIUGATION, UBIQUITIN-CONIUGATING ENZYME | UBIQUITIN CONJUGATION UBC2: UBIQUITIN CONJUGATION, UBIQUITIN-CONJUGATING ENZYME | LIGASE E6AP; UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN | LIGASE E6AP: UBCH7: BIL OBAL. | STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN | LIGASE UBIQUITIN, UBIQUITIN- | LIGASE UBIQUITIN, UBIQUITIN- | UBIQUITIN-CONTUGATING ENZYME UBIQUITIN-CONTUGATING ENZYME; | UBIQUITIN-CONJUGATING ENZYME, UBIQUITIN-DIRECTED 2 PROTEOLYSIS, CELL CYCLE CONTROL, LIGASE | UBIQUITIN-CONJUGATING ENZYME UBIQUITIN-CONJUGATING ENZYME; UBIQUITIN-CONJUGATING ENZYME, UBIQUITIN-DIRECTED 2 PROTED, YSIS, CELL CYCLE CONTROL 11GASE | UBIQUITIN CONJUGATION UBCI; | UBIQUITIN CONJUGATION UBCI; | UBIOUITIN CONJUGATION |
| Coumpound | CHAIN: A, B; | | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, C; | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, C: | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING PNZYMF F2: CHAIN: D. | I IBIOUITIN-PROTEIN | LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING | UBIQUITIN CONJUGATING | UBIQUITIN CONJUGATING FNZYME: CHAIN: A: | UBC9; CHAIN: NULL; | | UBC9; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME: CHAIN: NI I I | UBIQUITIN CONJUGATING ENZYME: CHAIN: NULL: | UBIQUITIN CONJUGATING |
| SeqFold score | | | | 90.32 | | 89.72 | | 87.99 | | 74.26 | | | | 93.12 | 81.53 |
| PMF | | | _ | | _ | | | | | | | L | _ | | |
| Verify | | | 0.49 | | 0.3 | | | | 9:0 | | | 0.17 | 0.38 | | |
| PSI- BLAST | | | 1.10E-45 | 1.10E-45 | 6.40E-39 | 6.40E-39 | | 9.60E-49 | 9.60E-49 | 9.60E-43 | | 9.60E-43 | 6.40E-48 | 6.40E-48 | 3.20E-44 |
| End | | | 157 | 171 | 157 | 166 | | 168 | 157 | 168 | | 157 | 157 | 148 | 156 |
| Start | | | 9 | 9 | 01 | 01 | | 7 | ® | 3 | | · . | 5 | 9 | _ |
| Chain D | - | | 4 | 4 | Д | ۵ | | V | V V | V | | < | | | |
| සු ස | | | layz | layz | 1c4z | Ic4z | | Iqcq | Гред | Iu9a | | lu9a | 2aak | 2aak | 2e2c |
| Š e Š | | | 882 | 882 | 882 | 882 | | 882 | 882 | 882 | | 882 | 882 | 882 | 882 |

| PDB annotation | UBIQUITIN CONTUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 BOND, LIGASE | UBIQUITIN CONJUGATION UBIQUITIN CONJUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 BOND, LIGASE | UBIQUITIN CONTUGATION UBC7; UBIQUITIN CONTUGATION, LIGASE, YEAST | UBIQUITIN CONIUGATION UBC7; UBIQUITIN CONIUGATION, LIGASE, YEAST | UBIQUITIN CONIUGATION UBC2; UBIQUITIN CONIUGATION, UBIQUITIN-CONIUGATING ENZYME | UBIQUITIN CONJUGATION UBC2; UBIQUITIN CONJUGATION, UBIQUITIN-CONJUGATING ENZYME | LIGÁSE E6AP; UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | LIGASE E6AP: UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | LIGASE UBIQUITIN, UBIQUITIN- CONJUGATING ENZYME, YEAST | LIGASE UBIQUITIN, UBIQUITIN- CONJUGATING ENZYME, YEAST | UBIQUITIN-CONUGATING ENZYME UBIQUITIN-CONUGATING ENZYME, UBIQUITIN-CONUGATING ENZYME, UBIQUITIN-CONUGATING ENZYME, UBIQUITIN-DIRECTED 2 PROTEOLY SIS, CELL CYCLE CONTROL, LIGASE | UBIQUITIN-CONJUGATING ENZYME UBIQUITIN-CONJUGATING ENZYME; UBIQUITIN-CONJUGATING ENZYME; UBIQUITIN-DIRECTED 2 |
|------------------|--|---|--|--|---|---|---|---|---|---|--|---|
| Coumpound | ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, C; | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, C: | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2; CHAIN: D; | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2; CHAIN: D; | UBIQUITIN CONJUGATING ENZYME; CHAIN: A; | UBIQUITIN CONJUGATING ENZYME; CHAIN: A; | UBC9; CHAIN: NULL; | UBC9; CHAIN: NULL; |
| SeqFold score | | | | 121.4 | 114.6 | | | 104.56 | 104.4 | | 94.76 | |
| PMF | | _ | - | | | _ | _ | | | _ | | 1 |
| Verify | | 0.27 | 0.63 | | | 0.73 | 0.4 | | | 0.53 | | 0.8 |
| PSI- BLAST | | 3.20E-44 | 3.20E-51 | 3.20E-51 | 6.40E-50 | 6.40E-50 | 3.20E-42 | 3.20E-42 | 1.10E-53 | 1.10E-53 | 4.80E-45 | 4.80E-45 |
| End AA | | 157 | 157 | 165 | 178 | 178 | 591 | 691 | 166 | 166 | 174 | 173 |
| Start AA | | 3 | 9 | 7 | 9 | 9 | 01 | 10 | 7 | ∞ | m | S |
| Chain | | | | | ¥ | ٧. | Ω | Q | ∢ | ∢ | < | ٧ |
| EDB CD | | 2e2c | 2ucz | 2ncz | layz | layz | lc4z | 1042 | lqcq | lqcq | 109a | Iu9a |
| S a S | | 882 | 882 | 882 | 882 | 882 | 882 | 882 | 882 | 882 | 882 | 882 |

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| PDB annotation | PROTEOLYSIS, CELL CYCLE CONTROL, LIGASE | UBIQUITIN CONJUGATION UBCI; UBIQUITIN CONJUGATION, LIGASE | UBIQUITIN CONJUGATION UBCI; UBIQUITIN CONJUGATION, LIGASE | UBIQUITIN CONJUGATION UBIQUITIN CONJUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 BOND, LIGASE | UBIQUITIN CONJUGATION UBIQUITIN CONJUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 BOND, LIGASE | UBIQUITIN CONJUGATION UBC7. UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC7; UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONTUGATION UBC2; UBIQUITIN CONTUGATION, UBIQUITIN-CONTUGATING ENZYME | LIGASE EKAP: UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | LIGASE E6AP: UBCH7; BLOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | LIGASE UBIQUITIN, UBIQUITIN- CONJUGATING ENZYME, YEAST | UBIQUITIN-CONUGATING ENZYME UBIQUITIN-CONUGATING ENZYME; UBIQUITIN-CONUGATING ENZYME; UBIQUITIN-CONUGATING ENZYME; UBIQUITIN-DIRECTED 2 PROTEDOLYSIS, CELL CYCLE CONTROL, LIGASE | UBIQUITIN CONJUGATION UBCI; UBIQUITIN CONJUGATION, LIGASE |
| Coumpound | | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONIUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME: CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, C; | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2; CHAIN: D; | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2: CHAIN: D: | UBIQUITIN CONJUGATING ENZYME: CHAIN: A: | UBC9; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; |
| SeqFold score | | | 116.78 | 109.63 | | | 148.79 | | | 51.09 | | | |
| PMF | | - | | | _ | _ | | 0.75 | 0.54 | | 9.0 | 0.72 | 0.55 |
| Verify score | | 0.62 | | | 0.55 | 0.59 | | 0.19 | -0.22 | | 0.2 | 0.18 | 90:0 |
| PSI- BLAST | | 8.00E-52 | 8.00E-52 | 1.60E-45 | 1.60E-45 | 1.60E-55 | 1.60E-55 | 4.80E-37 | 1.60E-28 | 1.60E-28 | 3.20E-39 | 3.20E-34 | 3.20E-38 |
| End AA | | 172 | 174 | 176 | 160 | 091 | 174 | 128 | 128 | 163 | 128 | 128 | 128 |
| Start AA | | 5 | 9 | _ | £ | 9 | 7 | 9 | 01 | 01 | ∞ | s | 5 |
| Chain ID | | | | | | | | V | D | D | ٧ | ⋖ | |
| PDB ID | | 2aak | 2aak | 2e2c | 2e2c | 2ucz | 2ucz | layz | 1c4z | 1c4z | Iqeq | lu9a | 2aak |
| SEQ ID NO: | | 882 | 882 | 882 | 882 | 882 | 882 | 882 | 882 | 882 | 882 | 882 | 882 |

| PDB annotation | UBIQUITIN CONJUGATION UBCI; UBIQUITIN CONJUGATION, LIGASE | UBIQUITIN CONIUGATION UBIQUITIN CONIUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 BOND, LIGASE | UBIQUITIN CONJUGATION UBC7; UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC7; UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC2; UBIQUITIN CONJUGATION, UBIQUITIN CONJUGATING ENZYME | UBIQUITIN CONJUGATION UBC2; UBIQUITIN CONJUGATION, UBIQUITIN-CONJUGATING ENZYME | LIGASE E6AP, UBCH7, BILOBAL STRUCTURE, ELONGATED SHAPE, E3 | UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | LIGASE E6AP, UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 | UBIQUITIN LIGASE, E2 2 UBIQUITIN CONTUGATING ENZYME | LIGASE UBIQUITIN, UBIQUITIN- CONJUGATING ENZYME, YEAST | LIGASE UBIQUITIN, UBIQUITIN- CONJUGATING ENZYME, YEAST | UBIQUITIN-CONJUGATING ENZYME | UBIQUITIN-CONJUGATING ENZYME, UBIQUITIN-CONJUGATING ENZYME, | UBIQUITIN-DIRECTED 2 | PROTEOLYSIS, CELL CYCLE CONTROL. LIGASE | UBIQUITIN-CONJUGATING ENZYME | UBIQUITIN-CONJUGATING ENZYME; | UBIQUITIN-DIRECTED 2 |
|-----------------|--|---|--|--|---|---|---|---|---|---|---|---|------------------------------|---|----------------------|---|------------------------------|-------------------------------|----------------------|
| Coumpound | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, C; | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, C: | UBIQUITIN-PROTEIN | UBIQUITIN CONJUGATING ENZYME E2; CHAIN: D; | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; | UBIQUITIN CONJUGATING ENZYME E2; CHAIN: D; | UBIQUITIN CONTUGATING ENZYME; CHAIN: A; | UBIQUITIN CONTUGATING ENZYME: CHAIN: A: | UBC9; CHAIN: NULL; | | | | UBC9; CHAIN: NULL; | - | |
| SeqFold | 50.62 | | | 56.09 | | 90.32 | | | 89.72 | | 87.99 | | 74.26 | | | | | | |
| PMF | | 0.25 | 0.49 | | _ | | _ | | | | | | | | | | _ | | |
| Verify score | | 0.17 | -0.09 | | 0.49 | | 0.3 | | | | | 9.0 | | | | | 0.17 | | |
| PSI- BLAST | 3.20E-38 | 1.10E-35 | 1.60E-35 | 1.60E-35 | 1.10E-45 | 1.10E-45 | 6.40E-39 | | 6.40E-39 | | 9.60E-49 | 9.60E-49 | 9.60E-43 | | | | 9.60E-43 | | |
| End | 155 | 126 | 128 | 136 | 157 | 171 | 157 | | 166 | | 891 | 157 | 168 | | | | 157 | | |
| Start | 9 | E . | 9 | 7 | 9 | 9 | 10 | | 10 | | 7 | | | | | | 5 | | |
| Chain D | | | | | A | ∢ | Q | | Q | | A | A | A | | | | V | | |
| 807 ED | 2aak | 2e2c | 2ncz | 2ucz | layz | layz | 1c4z | | 1c4z | | lqcq | Ided | Iu9a | | | | lu9a | | |
| S a S | 882 | 882 | 882 | 882 | 883 | 883 | 883 | | 883 | | 883 | 883 | 883 | | | | 883 | | |

| | | | | | | | | | , | | | | | |
|----------------|--|--|--|--|--|--|--|---|---|---|---|---|---|--|
| PDB annotation | PROTEOLYSIS, CELL CYCLE CONTROL, LIGASE | UBIQUITIN CONJUGATION UBCI; UBIQUITIN CONJUGATION, LIGASE | UBIQUITIN CONJUGATION UBCI; UBIQUITIN CONJUGATION, LIGASE | UBIQUITIN CONJUGATION UBIQUITIN CONJUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 BOND, LIGASE | UBIQUITIN CONJUGATION UBIQUITIN CONJUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 BOND, LIGASE | UBIQUITIN CONJUGATION UBC7; UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC7; UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONTUGATION UBC2; UBIQUITIN CONJUGATION, UBIQUITIN-CONJUGATING ENZYME | UBIQUITIN CONIUGATION UBC2, UBIQUITIN CONIUGATION, UBIQUITIN-CONIUGATING ENZYME | LIGASE E6AP: UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | LIGASE E6AP; UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | LIGASE UBIQUITIN, UBIQUITIN- CONIUGATING ENZYME, YEAST | LIGASE UBIQUITIN, UBIQUITIN- CONTUGATING ENZYME, YEAST | UBIQUITIN-CONJUGATING ENZYME UBIQUITIN-CONJUGATING ENZYME; UBIQUITIN-CONJUGATING ENZYME, |
| Coumpound | | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN-CONJUGATING ENZYME RAD6, CHAIN: A, B, C; | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, C; | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2; CHAIN: D; | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2; CHAIN: D; | UBIQUITIN CONJUGATING ENZYME; CHAIN: A; | UBIQUITIN CONJUGATING ENZYME; CHAIN: A; | UBC9; CHAIN: NULL; |
| SeqFold | | | 93.12 | 81.53 | | | 121.4 | 114.6 | | | 104.56 | 104.4 | | 94.76 |
| PMF | | _ | | | - | - | | | _ | _ | | | _ | |
| Verify | | 0.38 | | | 0.27 | 0.63 | | | 0.73 | 9.4 | | | 0.53 | |
| PSI- BLAST | | 6.40E-48 | 6.40E-48 | 3.20E-44 | 3.20E-44 | 3.20E-51 | 3.20E-51 | 6.40E-50 | 6.40E-50 | 3.20E-42 | 3.20E-42 | 1.10E-53 | 1.10E-53 | 4.80E-45 |
| End | | 157 | 148 | 156 | 157 | 157 | 165 | 178 | 8/1 | 591 | 691 | 991 | 99I | 174 |
| Start AA | | 5 | 9 | - | en en | 9 | 7 | 9 | 9 | 01 | 10 | 7 | ∞ | m · |
| Chain | | | | | | | | ¥- | A | D | Q | ¥ | ¥ | V |
| 908 10 | | 2aak | 2aak | 2e2c | 2e2c | 2ucz | 2ucz | layz | layz | 1042 | 1¢4z | Idcd | Iqcq | lu9a |
| SEQ BO: | | 883 | 883 | 883 | 883 | 883 | 883 | 883 | 883 | 883 | 883 | 883 | 883 | 883 |

| PDB annotation | UBIQUITIN-DIRECTED 2 PROTEOLYSIS, CELL CYCLE CONTROL, LIGASE | UBIQUITIN-CONJUGATING ENZYME UBIQUITIN-CONJUGATING ENZYME; UBIQUITIN-CONJUGATING ENZYME, | UBIQUITIN-DIRECTED 2 PROTEOLYSIS, CELL CYCLE CONTROL, LIGASE | UBIQUITIN CONJUGATION UBCI; UBIQUITIN CONJUGATION, LIGASE | UBIQUITIN CONJUGATION UBCI; UBIQUITIN CONJUGATION, LIGASE | UBIQUITIN CONTUGATION UBIQUITIN CONUGATION, UBIQUITIN CARRIER PROTEIN, THIORSTER 2 ROWN I GASE | UBIQUITIN CONUGATION UBIQUITIN CONUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 ROND. LIGASE | UBIQUITIN CONJUGATION UBC?; UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC7; UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC2; UBIQUITIN CONJUGATION, UBIQUITIN-CONJUGATING ENZYME | LIGASE E6AP; UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | LIGASE E6AP; UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | LIGASE UBIQUITIN, UBIQUITIN- CONJUGATING ENZYME, YEAST | UBIQUITIN-CONJUGATING ENZYME |
|------------------|--|--|--|--|--|--|--|--|--|---|---|--|---|------------------------------|
| Соитроинд | | UBC9; CHAIN: NULL; | | UBIQUITIN CONJUGATING ENZYME: CHAIN: NULL: | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONIUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYMB; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, C; | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2; CHAIN: D; | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2: CHAIN: D. | UBIQUITIN CONJUGATING ENZYME: CHAIN: A: | UBC9; CHAIN: NULL; |
| SeqFold score | | | | | 116.78 | 109.63 | | | 148.79 | | | 51.09 | | |
| PMF | | - | | _ | | - | ı | _ | | 0.75 | 0.54 | | 9.0 | 0.72 |
| Verify | | 8.0 | | 0.62 | | | 0.55 | 0.59 | | 0.19 | -0.22 | | 0.2 | -0.18 |
| PSI- BLAST | | 4.80E-45 | | 8.00E-52 | 8.00E-52 | 1.60E-45 | 1.60E-45 | 1.60E-55 | 1.60E-55 | 4.80E-37 | 1.60E-28 | 1.60E-28 | 3.20E-39 | 3.20E-34 |
| End | | 173 | | 172 | 174 | 176 | 160 | 091 | 174 | 128 | 128 | 163 | 128 | 128 |
| Start AA | | \$ | | 2 | 9 | | m | 9 | 7 | 9 | 01 | 01 | 8 | 5 |
| Chain | | ٧ | | | | | | | | ∢ | Ω | Ω | ٧ | A |
| PDB CI | | 1119a | | 2aak | Zaak | 2e2c | 2e2c | 2ucz | 2ucz | layz | 1c4z | 104z | Ided | 1u9a |
| SEQ B B S | | 883 | | 883 | 883 | . 883 | 883 | 883 | 883 | 883 | 883 | 883 | 883 | 883 |

| PDB annotation | UBIQUITIN-CONJUGATINO ENZYME; UBIQUITIN-CONJUGATINO ENZYME, UBIQUITIN-DIRECTED 2 PROTEOLYSIS, CELL CYCLE CONTROL, LIGASE | UBIQUITIN CONJUGATION UBCI; UBIQUITIN CONJUGATION, LIGASE | UBIQUITIN CONTUGATION UBCI; UBIQUITIN CONTUGATION, LIGASE | UBIQUITIN CONJUGATION UBIQUITIN CONJUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 BOND, LIGASE | UBIQUITIN CONTUGATION UBC7; UBIQUITIN CONTUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC7; UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC2; UBIQUITIN CONJUGATION, UBIQUITIN-CONJUGATING ENZYME | UBIQUITIN CONJUGATION UBC2; UBIQUITIN CONJUGATION, | UBIQUITIN-CONJUGATING ENCYME | LÍGASE EGAP: UBCH7: BILOBAL. STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LÍGASE, E2 2 UBIQUITIN CONUGATING ENZYME | LIGASE E6AP; UBCH7; BILOBAL | STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | LIGASE UBIQUITIN, UBIQUITIN- | LIGASE UBIQUITIN, UBIQUITIN- CONILIGATING ENZYME YEAST | UBIQUITIN-CONJUGATING ENZYME: UBIQUITIN-CONJUGATING ENZYME; UBIQUITIN-CONJUGATING ENZYME, |
|-----------------|--|--|--|---|--|--|---|---|------------------------------|---|-----------------------------|--|---|---|---|
| Coumpound | | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN-CONJUGATING ENZYME RAD6: CHAIN: A. B, C: | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, | ני | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2; CHAIN: D; | UBIQUITIN-PROTEIN | LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2: CHAIN: D: | UBIQUITIN CONJUGATING ENZYME: CHAIN: A | UBIQUITIN CONJUGATING ENZYME: CHAIN: A: | UBC9; CHAIN: NULL; |
| SeqFold | | | 50.62 | | | 56.09 | | 90.32 | | | 89.72 | | 87.99 | | 74.26 |
| PMF | | 0.55 | | 0.25 | 0.49 | | _ | | | _ | | | | _ | |
| Verify score | | 90.0 | | 0.17 | -0.09 | | 0.49 | | | 6.3 | | | | 9.0 | |
| PSI- BLAST | | 3.20E-38 | 3.20E-38 | 1.10E-35 | 1.60E-35 | 1.60E-35 | 1.10E-45 | 1.10E-45 | | 6.40E-39 | 6.40E-39 | | 9.60E-49 | 9.60E-49 | 9.60E-43 |
| End | | 128 | 155 | 126 | 128 | 136 | 157 | 171 | 1 | 157 | 991 | | 891 | 157 | 168 |
| Start AA | | 5 | 9 | 3 | 9 | | 9 | 9 | | <u>.</u> | 10 | | 7 | ∞ | 3 |
| Chain | | | | | | | ∢ | 4 | Ī, | ď | Q | | ¥ | V | V V |
| PDB | | 2aak | 2aak | 2e2c | 2ncz | 2ncz | layz | Iayz | 1 | lc4z | 1c4z | | ldcd | Idea | Iu9a |
| SEQ NO: O | | 883 | 883 | 883 | 883 | 883 | 884 | 884 | | 884 | 884 | | 884 | 884 | 884 |

| PDB annotation | UBIQUITIN-DIRECTED 2 PROTEOLYSIS, CELL CYCLE CONTROL, LIGASE | UBIQUITIN-CONUGATING ENZYME UBIQUITIN-CONUGATING ENZYME, UBIQUITIN-CONUGATING ENZYME, UBIQUITIN-DIRECTED 2 PROTEOLYSIS, CELL CYCLE CONTROL 112ASE | UBIQUITIN CONJUGATION UBC1; UBIOUITIN CONJUGATION, LIGASE | UBIQUITIN CONJUGATION UBC1; UBIQUITIN CONJUGATION, LIGASE | UBIQUITIN CONJUGATION UBIQUITIN CONJUGATION, UBIQUITIN CARRIER PROTEIN, THIORSTER 2 BOND LIGASE | UBIQUITIN CONJUGATION UBIQUITIN CONJUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 BOND. LIGASE | UBIQUITIN CONJUGATION UBC7; UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC7: UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC2; UBIQUITIN CONJUGATION, UBIQUITIN-CONJUGATING ENZYME | UBIQUITIN CONJUGATION UBC2; UBIQUITIN CONJUGATION, | LIGASE E6AP; UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, B3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONILIGATING ENZYME | LIGASE EGAP; UBCH; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 UBIQUITIN CONJIGATING PAYZYAR |
|------------------|--|---|--|--|---|--|--|--|---|--|--|---|
| Coumpound | | UBC9; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME: CHAIN: NULL: | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME, CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, C: | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, C: | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2: CHAIN: D: | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYMF E2: CHAIN: D. |
| SeqFold score | | | | 93.12 | 81.53 | | | 121.4 | 114.6 | | | 104.56 |
| PMF | | _ | _ | | | _ | - | | | _ | - | |
| Verify score | | 0.17 | 0.38 | | | 0.27 | 0.63 | | | 0.73 | 0.4 | |
| PSI- BLAST | | 9.60E-43 | 6.40E-48 | 6.40E-48 | 3.20E-44 | 3.20E-44 | 3.20E-51 | 3.20E-51 | 6.40E-50 | 6.40E-50 | 3.20E-42 | 3.20E-42 |
| End | | 157 | 157 | 148 | 156 | 157 | 157 | 165 | 178 | 178 | 165 | 169 |
| Start AA | | S | 5 | 9 | 1 | E . | 9 | | 9 | 9 | .01 | 10 |
| Chain ID | | Y | | | | | | | ٧ | ¥ | Q | Q |
| PDB DD | | Iu9a | 2aak | 2aak | 2620 | 2e2c | 2ucz | 2ucz | layz | layz | lo4z | lc4z |
| SEQ No: | | 884 | 884 | 884 | 884 | 884 | 884 | 884 | 884 | 884 | 884 | 884 |

| | | | | | | | | | | | _ | |
|------------------|---|---|---|---|---|--|--|--|--|--|---|---|
| PDB annotation | LIGASE UBIQUITIN, UBIQUITIN- CONTUGATING ENZYME, YEAST | LIGASE UBIQUITIN, UBIQUITIN- CONJUGATING ENZYME. YEAST | UBIQUITIN-CONIDGATNG ENZYME UBIQUITIN-CONIDGATNG ENZYME, UBIQUITIN-CONIUGATNG ENZYME, UBIQUITIN-DIRECTED 2 PROTEOLYSIS, CELL CYCLE CONTROL_LIGASE | UBIQUITIN-CONIUGATING ENZYME UBIQUITIN-CONIUGATING ENZYME, UBIQUITIN-CONIUGATING ENZYME, UBIQUITIN-DIRECTED 2 PROTIED/SIS, CELL CYCLE CONTROL, 11GAST | UBIQUITIN CONJUGATION UBCI; | UBIQUITIN CONJUGATION UBCI; IJBIQUITIN CONJUGATION LIGASE | UBIQUITIN CONTUGATION UBIQUITIN CONTUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 BOND, LIGASE | UBIQUITIN CONJUGATION UBIQUITIN CONJUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 BOND, LIGASE | UBIQUITIN CONJUGATION UBC7; UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC7; UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC2; UBIQUITIN CONJUGATION, | LIGASE EGAP, UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME |
| Coumpound | UBIQUITIN CONJUGATING ENZYME, CHAIN: A; | UBIQUITIN CONJUGATING ENZYME; CHAIN: A; | UBC9; CHAIN: NULL; | UBC9; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME: CHAIN: NITL: | UBIQUITIN CONJUGATING ENZYME: CHAIN: NULL: | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN-CONJUGATING ENZYME RAD6; CHAIN: A, B, | ÚBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2; CHAIN: D; |
| SeqFold score | 104.4 | | 94.76 | | | 116.78 | 109.63 | | | 148.79 | | |
| PMF score | | _ | | - | - | | | _ | 1 | | 0.75 | 0.54 |
| Verify | | 0.53 | | 8.0 | 0.62 | | | 0.55 | 0.59 | | 0.19 | -0.22 |
| PSI- BLAST | 1.10E-53 | 1.10E-53 | 4.80E-45 | 4.80E-45 | 8.00E-52 | 8.00E-52 | 1.60E-45 | 1.60E-45 | 1.60E-55 | 1.60E-55 | 4.80E-37 | 1.60E-28 |
| End | 991 | 991 | 174 | 173 | 172 | 174 | 9/1 | 160 | 160 | 174 | 128 | 128 |
| Start | 7 | 8 | m | ۶ | | 9 | _ | 3 | 9 | 7 | 9 | 01 |
| Chain D | Ą | A | ∢ | ٧ | | - | | | | | ٧ | Д |
| PDB ID | 1qcq | Iqcq | lu9a | lu9a | 2aak | 2aak | 2e2c | 2e2c | 2ucz | 2ucz | layz | 1042 |
| SEQ NO: | 884 | 884 | 884 | 884 | 884 | 884 | 884 | 884 | 884 | 884 | 884 | 884 |

| PDB annotation | LIGASE E6AP; UBCH7; BILOBAL STRUCTURE, ELONGATED SHAPE, E3 UBIQUITIN LIGASE, E2 2 UBIQUITIN CONJUGATING ENZYME | LIGASE UBIQUITIN, UBIQUITIN- CONJUGATING ENZYME, YEAST | UBIQUITIN-CONUGATING BRZYME UBIQUITIN-CONUGATING BRZYME, UBIQUITIN-CONUGATING BRZYME, UBIQUITIN-DIRECTED 2 PROTEOLYSIS, CELL CYCLE CONTROL, LIGABE | UBIQUITIN CONJUGATION UBCI; UBIQUITIN CONJUGATION, LIGASE | UBIQUITIN CONJUGATION UBCI; UBIQUITIN CONJUGATION, LIGASE | UBIQUITIN CONJUGATION UBIQUITIN CONJUGATION, UBIQUITIN CARRIER PROTEIN, THIOESTER 2 BOND, LIGASE | UBIQUITIN CONJUGATION UBC7; UBIQUITIN CONJUGATION, LIGASE, YEAST | UBIQUITIN CONJUGATION UBC7; UBIQUITIN CONJUGATION, LIGASE, YEAST | LIPID TRANSPORT APO A-1: LIPOPROTEIN, LIPID TRANSPORT, CHOLESTEROL METABOLISM, 2 ATHEROSCLEROSIS, HDL, LCAT- ACTIVATION | HYDROLASE ERA, GTPASE, RNA- BINDING, RAS-LIKE, HYDROLASE | TRANSLATION TRANSLATIONAL GTPASE | CONTRACTILE PROTEIN TRIPLE- HELIX COILED COIL, CONTRACTILE PROTEIN | HUMAN SKELETAL MUSCLE CONTRACTILE PROTEIN TRIPLE- |
|----------------|---|---|--|--|--|---|--|--|---|---|---|--|---|
| Coumpound | UBIQUITIN-PROTEIN LIGASE E3A; CHAIN: A, B, C; UBIQUITIN CONJUGATING ENZYME E2; CHAIN: D; | UBIQUITIN CONJUGATING ENZYME; CHAIN: A; | UBC9; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | UBIQUITIN CONJUGATING ENZYME; CHAIN: NULL; | APOLIPOPROTEIN A-1; CHAIN: A, B, C, D; | GTP-BINDING PROTEIN ERA; CHAIN: A. B: | TRANSLATION INITIATION FACTOR IFZEIF5B; CHAIN: A: | HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A: | HUMAN SKELETAL MUSCLE |
| SeqFold | 51.09 | | | | 50.62 | | | 56.09 | 53.53 | | | | |
| PMF | | 9.0 | 0.72 | 0.55 | | 0.25 | 0.49 | | | 0.01 | 0.03 | 10:0- | -0.01 |
| Verify | | 0.2 | 91.0- | 90:0 | | 0.17 | -0.09 | | | -0.14 | -0.34 | 0.23 | 0.23 |
| PSI- BLAST | 1.60E-28 | 3.20E-39 | 3.20E-34 | 3.20E-38 | 3.20E-38 | 1.10E-35 | 1.60E-35 | 1.60E-35 | 5.40E-07 | 1.60E-37 | 6.40E-06 | 1.80E-08 | 1.80E-08 |
| End | 163 | 128 | 128 | 128 | 155 | 126 | 128 | 136 | 427 | 350 | 289 | 426 | 445 |
| Start | . 01 | | s | 2 | 9 | æ | 9 | 7 | 237 | 39 | 45 | 283 | 302 |
| Chain ID | Д | ٧ | < | | | | | | ⋖ | ∢ | ∀ | ∢ | A |
| PDB DD | lc4z | lqcq | lu9a | 2aak | 2aak | 2e2c | 2ucz | 2ucz | lavI | lega | 187s | Iquu | 1quu |
| S e Š | 884 | 884 | 288 | 884 | 884 | 884 | 884 | 884 | 882 | \$85 | 885 | 885 | 885 |

| PDB annotation | HELIX COILED COIL, CONTRACTILE PROTEIN | LIPID TRANSPORT APO A-1; LIPOPROTEIN, LIPID TRANSPORT, CHOLESTEROL METABOLISM, 2 ATHEROSCLEROSIS, HDL, LCAT- | HYDROLASE ERA, GTPASE, RNA- BINDING, RAS-LIKE, HYDROLASE | TRANSLÁTION TRANSLATIONAL GTPASE | CONTRACTILE PROTEIN TRIPLE- HELIX COILED COIL, CONTRACTILE PROTEIN | CONTRACTILE PROTEIN TRIPLE. HELIX COILED COIL, CONTRACTILE PROTEIN | | IMMUNOGLOBULIN IMMUNOGLOBULIN, KAPPA LIGHT- CHAIN DIMER HEADER | COMPLEX (ANTIBODY/ANTIGEN) FAB-12: VEGF; COMPLEX (ANTIBODY/ANTIGEN), ANGIOGENIC FACTOR | COMPLEX (HUMANIZED ANTIBODYHTDROLASE) ANTIBODY, ANTIBODY COMPLEX, FV, ANTI-YSOZYME, 2 COMPLEX (HUMANIZED ANTIBODY, ANTIBODY COMPLEX ANTIBODY ANTIBODY COMPLEX (HUMANIZED | IMMUNE SYSTEM REIV, STABILIZED IMMUNGLOBULIN FRAGMENT, BENCE-JONES 2 PROTEIN, IMMUNE SYSTEM | IMMUNE SYSTEM FAB-IBP COMPLEX CRYSTAL STRUCTURE 2.7A RESOLUTION BINDING 2 OUTSIDE |
|-----------------|--|--|---|---|--|--|---|--|--|--|---|---|
| Coumpound | ALPHA-ACTININ 2; CHAIN: A; | APOLIPOPROTEIN A-1; CHAIN: A, B, C, D; | GTP-BINDING PROTEIN ERA; CHAIN: A. B: | TRANSLATION INITIATION FACTOR IFZEIF5B; CHAIN: A: | HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A: | HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A; | | IMMUNOGLOBULIN; CHAIN: A, B; | FAB FRAGMENT; CHAIN: L, H, J, K; VASCULAR ENDOTHELIAL GROWTH FACTOR: CHAIN: V, W; | HULYSU; CHAIN: A, B, D, E; -LYSOZYME; CHAIN: C, F; | IG KAPPA CHAIN V-I REGION REI; CHAIN: A, B; | IGM RF 2A2; CHAIN: A, C, E; IGM RF 2A2; CHAIN: B, D, F; IMMUNOGLOBULIN G |
| SeqFold | | 53.53 | | | | | | | | | | |
| PMF | | | 0.01 | 0.03 | -0.01 | -0.01 | | 0.17 | 0.11 | -0.09 | 0.34 | .0.1 |
| Verify score | | | -0.14 | -0.34 | 0.23 | 0.23 | | 0.2 | 0.13 | 0.18 | 0.15 | -0.2 |
| PSI- BLAST | | 5.40E-07 | 1.60E-37 | 6.40E-06 | 1.80E-08 | 1.80E-08 | | 3.20E-41 | 3.20E-43 | I.60E-42 | 4.80E-43 | 3.20E-43 |
| End | | 427 | 320 | 289 | 426 | 445 | | 811 | 116 | 611 | 8 1 | 115 |
| Start | | 237 | 39 | 45 | 283 | 302 | | 61 | 61 | 19 | 61 | 19 |
| Chain | | ¥ | V | A | V | 4 | | ٧ | 1 | ∢ | ¥ | ¥ |
| 80 e | | lavl | lega | lg7s | lquu | Iqua | | p9qI | 161 | Ibvk | wd! w | 1dee |
| SEQ No es | | 988 | 988 | 988 | 988 | 988 | ĺ | 887 | 887 | 887 | 887 | 887 |

| | | | | | | _ | | | | | |
|-----------------|---|--|--|--|--|---|--|---|---|--|---|
| PDB annotation | THE ANTIGEN COMBINING SITE SUPERANTIGEN FAB VH3 3 SPECIFICITY | | | IMMUNOGLOBULIN TR.1.9, ANTI- THYROID PEROXIDASE, AUTOANTIBODY, 2 IMMUNOGLOBULIN | | | DNA-BINDING PROTEIN ISL-1HD DNA-BINDING PROTEIN, HOMEODOMAIN, LIM DOMAIN | COMPLEX (DNA-BINDING PROTEIN/DNA) DNA-BINDING PROTEIN, DNA, PAIRED BOX, TRANSCRIPTION 2 REGULATION | COMPLEX (DNA-BINDING PROTEIN/DNA) DNA-BINDING PROTEIN, DNA, PAIRED BOX, TRANSCRIPTION 2 REGULATION | COMPLEX (DNA-BINDING PROTEINDNA) DNA-BINDING PROTEIN, DNA, PAIRED BOX, TRANSCRIPTION 2 REGULATION | COMPLEX (DNA-BINDING PROTEIN/DNA) DNA-BINDING PROTEIN, DNA, PAIRED BOX, |
| Coumpound | BINDING PROTEIN A; CHAIN: G. H: | IMMUNOGLOBULIN FV FRAGMENT OF A HUMANIZED VERSION OF THE ANTI-CD18 IFGV 3 ANTIBODY 'H52' (HUH52-AA FV) IFGV 4 | IMMUNOGLOBULIN IMMUNOGLOBULIN M (IG- M) FV FRAGMENT IIGM 3 | TRI.9 FAB; CHAIN: L, H; | IMMUNOGLOBULIN FAB FRAGMENT OF A HUMANIZED VERSION OF THE ANTI-CD18 2FQW 3 ANTIBODY 'H32' (HUH52-OZ FAB) 2FGW 4 | | INSULIN GENE ENHANCER PROTEIN ISL-1; CHAIN: NULL; | PAIRED PROTEIN; CHAIN: A, B, C, DNA; CHAIN: D, E, F | PAIRED PROTEIN; CHAIN: A, B. C; DNA; CHAIN: D, E, F | PAIRED PROTEIN; CHAIN: A, B, C; DNA; CHAIN: D, E, F | PAIRED PROTEIN; CHAIN: A, B, C; DNA; CHAIN: D, E, F |
| SeqFold | | | | | | | | | 76.5 | 72.69 | |
| PMF | | 0.13 | -0.06 | 0.23 | 0.1 | | 0.42 | 1 | | | 1 |
| Verify score | | 0.31 | 0 | 0.15 | 0.32 | | 0.14 | 0.28 | | | 0.02 |
| PSI- BLAST | | 3.20E-44 | 1.40E-42 | 6.40E-41 | 1.60E-44 | | 9.00E-31 | 1.10E-28 | 1.10E-28 | 9.00E-28 | 9.00E-28 |
| End | | 911 | 125 | 118 | 116 | | 275 | 275 | 280 | 273 | 274 |
| Start | | 61 | 61 | 22 | 61 | | 216 | 216 | 216 | 217 | 21.7 |
| Chain | | <u>, </u> | ı | 1 | IJ | | | ٧ | ∀ | മ | В |
| PDB ID | | rĝji | 11gm | 1vge | 2fgw | | Ibw S | 161 | 191 | <u>1</u> 91 | 161 |
| S a S | | 887 | 887 | 887 | 887 | | 888 | 888 | 888 | 888 | 888 |

| | _ | | | | | | | | |
|----------------|----------------------------|--|---|---|---|--|--|--|---|
| PDB annotation | TRANSCRIPTION 2 REGULATION | COMPLEX (GENE REGULATING PROTEINDA) PAX, PRD, PAIRED DOMAIN, DNA-BINDING PROTEIN IPDN 14 | COMPLEX (GENE REGULATING PROTEINIDNA) PAX, PRD, PAIRED DOMAIN, DNA-BINDING PROTEIN IPDN 14 | COMPLEX (GENE REGULATING PROTEIN/DNA) PAX, PRD, PAIRED DOMAIN, DNA-BINDING PROTEIN IPDN 14 | DNA-BINDING DNA-BINDING, TRANSCRIPTION FACTOR, LFBI/HNFI, 2 HELIX,-TURN-HELIX, DNA-BINDING DOMAIN | GENE REGULATION/DNA PAX, PAIRED DOMAIN, TRANSCRIPTION, PROTEIN-DNA INTERACTIONS, 2 GENE REGULATION/DNA | GENE REGULATION/DNA PAX, PAIRED DOMAIN, TRANSCRIPTION, PROTEIN-DNA INTERACTIONS, 2 GENE REGULATION/DNA | GENE REGULATION/DNA PAX, PAIRED DOMAIN, TRANSCRIPTION, PROTEIN-DNA INTERACTIONS, 2 GENE REGULATION/DNA | |
| Coumpound | | PRD PAIRED DOMAIN; CHAIN: C; IPDN 4 DNA; CHAIN: A, B IPDN 5 | PRD PAIRED DOMAIN; CHAIN: C; IPDN 4 DNA; CHAIN: A, B IPDN 5 | PRD PAIRED DOMAIN; CHAIN: C; IPDN 4 DNA; CHAIN: A, B IPDN 5 | LFBJ/HNFI TRANSCRIPTION FACTOR; CHAIN: NULL; | HOMEOBOX PROTEIN PAX- 6; CHANI: A; 26 NUCLEOTIDE DNA; CHAIN: B; 26 NUCLEOTIDE DNA; CHAIN: C; | HOMEOBOX PROTEIN PAX. 6; CHAIN: A; 26 NUCLEOTIDE DINA; CHAIN: B; 26 NUCLEOTIDE DINA; CHAIN: C; | HOMEOBOX PROTEIN PAX- 6; CHAIN. A; 26 NUCLEOTIDE DNA; CHAIN: B; 26 NUCLEOTIDE DNA; CHAIN: C; | |
| SeqFold | | | 168.62 | | | 143.36 | | | |
| PMF | | _ | | _ | 0.33 | | | - | |
| Verify | | 0.57 | , | 0.66 | 0.31 | | 0.61 | 0.48 | |
| PSI- BLAST | | 9.60E-29 | 1.10E-63 | 1.10E-63 | 1.40E-30 | 1.60 <u>E-67</u> | 1.60E-31 | 1.60E-67 | |
| End | | 152 | 160 | 091 | 280 | 691 | 152 | 169 | |
| Start | | . 35 | 35 | 35 | 209 | 34 | 35 | 36 | |
| Chain ID | | ၁ | ပ | ပ | | ¥ | ∢ | ٧ | |
| PDB ID | | 1pdn | nbq! | nbq! | 2169 | брах | брах | брах | ٦ |
| SEQ NO: | | 888 | 888 | 888 | 888 | 88 | 888 | 888 | |

TABLE 6

| SEQ ID NO: | Position of Last Amino Acid of Signal Peptide | Maximum Score | Mean Score |
|------------|--|---------------|------------|
| 445 | 21 | 0.993 | 0.931 |
| 446 | 14 | 0.975 | 0.962 |
| 447 | 42 | 0.986 | 0.606 |
| 448 | 18 | 0.908 | 0.703 |
| 449 | | 0.967 | 0.778 |
| 450 | 30 | 0.992 | 0.946 |
| 452 | 17 | 0.997 | 0.973 |
| 454 | 32 | 0.907 | 0.575 |
| 455 | 27 | 0.931 | 0.672 |
| 456 | 40 | 0.988 | 0.755 |
| 457 | 26 | 0.986 | 0.916 |
| 458 | 18 | 0.920 | 0.750 |
| 459 | 15 | 0.946 | 0.790 |
| 460 | 21 | 0.993 | 0.931 |
| 461 | 47 | 0.942 | 0.644 |
| 463 | 24 | 0.886 | 0.712 |
| 464 | 36 | 0.985 | 0.712 |
| | | | |
| 465 | 42 | 0.965 | 0.679 |
| 466 | 2.3 | 0.980 | 0.946 |
| 467 | 27 | 0.969 | 0.858 |
| 469 | 26 | 0.950 | 0.793 |
| 470 | 45 | 0.983 | 0.687 |
| 471 | 25 | 0.981 | 0.821 |
| 472 | 30 | 0.998 | 0.963 |
| 473 | 18 | 0.977 | 0.915 |
| 474 | 27 | 0.949 | 0.644 |
| 475 | 23 | 0.913 | 0.768 |
| 476 | 19 | 0.947 | 0.901 |
| 477 | 15 | 0.936 | 0.628 |
| 478 | 17 | 0.956 | 0.893 |
| 479 | 17 | 0.942 | 0.720 |
| 480 | 19 | 0.952 | 0.730 |
| 481 | 17 | 0.970 | 0.916 |
| 483 | 14 | 0.975 | 0.962 |
| 486 | 47 | 0.955 | 0.727 |
| 488 | 23 | 0.991 | 0.952 |
| 495 | 42 | 0.986 | 0.606 |
| 496 | 11 | 0.971 | 0.594 |
| 502 | 29 | 0.896 | 0.743 |
| 509 | 18 | 0.908 | 0.703 |
| 510 | 13 | 0.959 | 0.908 |
| 512 | 20 | 0.957 | 0.858 |
| 516 | 24 | 0.967 | 0.778 |
| 517 | 35 | 0.991 | 0.851 |
| 518 | 26 | 0.939 | 0.722 |
| 519 | 47 | 0.983 | 0.640 |
| 522 | 30 | 0.992 | 0.946 |
| 538 | 16 | 0.974 | 0.924 |
| 550 | 17 | 0.997 | 0.973 |
| 551 | 42 | 0.947 | 0.588 |
| 555 | 30 | 0.947 | 0.684 |
| 576 | 30 | 0.981 | 0.575 |
| 577 | 26 | 0.907 | 0.927 |
| 578 | 26 | 0.973 | 0.672 |
| 589 | 40 | 0.931 | 0.755 |
| | | | |
| 590 | 38 | 0.985 | 0.775 |

| 595 | 20 | 0.938 | 0.818 |
|------------|-------|----------------|----------------|
| 611 | 18 | 0.920 | 0.750 |
| 615 | 25 | 0.949 | 0.775 |
| 616 | 33 | 0.995 | 0.835 |
| 617 | 15 | 0.946 | 0.790 |
| 623 | 19 | 0.921 | 0.819 |
| 627 | 21 | 0.993 | 0.931 |
| 634 | 20 | 0.961 | 0.674 |
| 635 | 28 | 0.954 | 0.648 |
| 645 | 47 | 0.942 | 0.644 |
| 647 | 31 | 0.962 | 0.776 |
| 650 | 16 | 0.949 | 0.782 |
| 651 | 14 | 0.963 | 0.613 |
| 654 | 20 | 0.984 | 0.958 |
| 670 | 24 | 0.886 | 0.712 |
| 673 | 17 | 0.934 | 0.753 |
| 678 | 36 | 0.985 | 0.865 |
| 695 | 23 | 0.954 | 0.754 |
| 707 | 42 | 0.965 | 0.679 |
| 708 | 2 | 0.979 | 0.667 |
| 709 | 24 | 0.984 | 0.851 |
| 710 | 17 | 0.911 | 0.745 |
| 717 | 25 | 0.980 | 0.946 |
| 718 | 35 | 0.988 | 0.871 |
| 726 | 27 | 0.969 | 0.858 |
| 730 | 17 | 0.981 | 0.844 |
| 741 | 22 | 0.937 | 0.871 |
| 755 | 17 | 0.890 | 0.668 |
| 764 | 26 | 0.950 | 0.793 |
| 768 | 32 | 0.958 | 0.827 |
| 771 | 45 | 0.983 | 0.687 |
| 773 | 39 | 0.997 | 0.801 |
| 776 | 17 | 0.945 | 0.650 |
| 787 | 32 | 0.983 | 0.835 |
| 789 | 25 | 0.981 | 0.821 |
| 792 | 31 | 0.966 | 0.815 |
| 796 | 22 | 0.887 | 0.572 |
| 797 | 19 | 0.941 | 0.691 |
| 807 | 30 | 0.998 | 0.963 |
| 808 | 18 | 0.977 | 0.915 |
| 809 | 18 | 0.977 | 0.915 |
| 811 | | 0.959 | 0.827 |
| 812 | 16 | 0.925 | 0.734 |
| 815 | 19 | 0.934 | 0.564 |
| 816 818 | 21 27 | 0.960 0.949 | 0.858 0.644 |
| | 27 | 0.949 | |
| 821 | | | 0.758 0.728 |
| 823 | 27 | 0.908 | |
| 833 | 23 | 0.913 | 0.768 |
| 837 | 19 | 0.947 0.967 | 0.901 0.826 |
| 841 845 | | | |
| | 15 | 0.936 | 0.628 |
| 846 | | 0.975 | 0.840 |
| 851 | 31 | 0.985 | 0.908 |
| 852 | 19 | 0.965 | 0.922 |
| 853 | 39 | 0.984 | 0.743 |
| 857 | r 17 | 0.956 | 0.893 |
| 858 | 21 | 0.957 | 0.868 |
| 861 | 22 | 0.975 | 0.866 |
| 868 | 21 | 0.942 | . 0.736 |

| 871 | 43 | 0.973 | 0.560 |
|-----|----|-------|-------|
| 873 | 19 | 0.952 | 0.730 |
| 874 | 33 | 0.923 | 0.717 |
| 879 | 23 | 0.978 | 0.911 |
| 881 | 16 | 0.947 | 0.884 |
| 887 | 17 | 0.970 | 0.916 |

TABLE 7

| SEQ ID NO: | Position of Last Amino Acid of Signal Peptide | Maximum Score | Mean Score |
|------------|--|----------------|----------------|
| 445 | 21 | 0.993 | 0.931 |
| 446 | 14 | 0.975 | 0.962 |
| 447 | 42 | 0.986 | 0.606 |
| 448 | 18 | 0.908 | 0.703 |
| 449 | 24 | 0.967 | 0.778 |
| 450 | 30 | 0.992 | 0.946 |
| 452 | 17 | 0.997 | 0.973 |
| 454 | 32 | 0.907 | 0.575 |
| 455 | 27 | 0.931 | 0.672 |
| 456 | 40 | 0.988 | 0.755 |
| 457 | 26 | 0.986 | 0.916 |
| 458 | 18 | 0.920 | 0.750 |
| 459 | 15 | 0.946 | 0.790 |
| 460 | 21 | 0.993 | 0.931 |
| 461 | 47 | 0.942 | 0.644 |
| 463 | 24 | 0.886 | 0.712 |
| 464 | 36 | 0.985 | 0.865 |
| 465 | 42 | 0.965 | 0.679 |
| 466 | 25 | 0.980 | 0.946 |
| 467 | 27 | 0.969 | 0.858_ |
| 469 | 26 | 0.950 | 0.793 |
| 470 | 45 | 0.983 | 0.687 |
| 471 | 25 | 0.981 | 0.821 |
| 472 | 30 | 0.998 | 0.963 |
| 473 | 18 | 0.977 | 0.915 |
| 474 | 27 | 0.949 | 0.644 |
| 475 | 23 | 0.913 | 0.768 |
| 476 | 19 | 0.947 | 0.901 |
| 477 | 15 | 0.936 | 0.628 |
| 478 | 17 | 0.956 | 0.893 · |
| 479 | 17 | 0.942 | 0.720 |
| 480 | 19 | 0.952 | 0.730 |
| 481 483 | 17 | 0.970 0.975 | 0.916 |
| 485 | 47 | | 0.962 0.727 |
| 488 | 23 | 0.955 0.991 | 0.727 |
| 495 | 42 | 0.991 | 0.606 |
| 496 | | 0.971 | 0.594 |
| 502 | 11 29 | 0.896 | 0.743 |
| 509 | 18 | 0.896 | 0.743 |
| 510 | 18 | 0.959 | 0.703 |
| 512 | 20 | 0.957 | 0.858 |
| 516 | 24 | 0.967 | 0.838 |
| 517 | 35 | 0.991 | 0.851 |
| 518 | 26 | 0.939 | 0.722 |
| 519 | 47 | 0.983 | 0.640 |
| 522 | 30 | 0.992 | 0.946 |
| 538 | 16 | 0.992 | 0.924 |
| 550 | 17 | 0.997 | 0.973 |
| 551 | 42 | 0.947 | 0.588 |
| 555 | 30 | 0.981 | 0.684 |
| 576 | 32 | 0.907 | 0.575 |
| 577 | 26 | 0.973 | 0.927 |
| 578 | 27 | 0.931 | 0.672 |
| 589 | 40 | 0.988 | 0.755 |

| 590 | 38 | 0.985 | 0.775 |
|------------|----------|----------------|----------------|
| 595 | 20 | 0.938 | 0.818 |
| 611 | 18 | 0.920 | 0.750 |
| 615 | 25 | 0.949 | 0.775 |
| 616 | 33 | 0.995 | 0.835 |
| 617 | 15 | 0.946 | 0.790 |
| 623 | 19 | 0.921 | 0.819 |
| 627 | 21 | 0.993 | 0.931 |
| 634 | 20 | 0.961 | 0.674 |
| 635 | 28 | 0.954 | 0.648 |
| 645 | 47 | 0.942 | 0.644 |
| 647 | 31 | 0.962 | 0.776 |
| 650 | 16 | 0.949 | 0.782 |
| 651 | 14 | 0.963 | 0.613 |
| 654 | 20 | 0.984 | 0.958 |
| 670 | 24 | 0.886 | 0.712 |
| 673 | 17 | 0.934 | 0.753 |
| 678 | 36 | 0.985 | 0.865 |
| 695 | 23 | 0.954 | 0.754 |
| 707 | 42 | 0.965 | 0.679 |
| 708 | 2 | 0.979 | 0.667 |
| 709 | 24 | 0.984 | 0.851 |
| 710 | 17 | 0.911 | 0.745 |
| 717 | 25 | 0.980 | 0.946 |
| 718 | 35 | 0.988 | 0.871 |
| 726 | 27 | 0.969 | 0.858 |
| 730 | 17 | 0.981 | 0.844 |
| 741 | 22 | 0.937 | 0.871 |
| 755 | 17 | 0.890 | 0.668 |
| 764 | 26 | 0.950 | 0.793 |
| 768 | 32 | 0.958 | 0.827 |
| 771 | 45 | 0.983 | 0.687 |
| 773 | 39 | 0.997 | 0.801 |
| 776 | 17 | 0.945 | 0.650 |
| 787 | 32 | 0.983 | 0.835 |
| 789 | 25 | 0.981 | 0.821 |
| 792 | 31 | 0.966 | 0.815 |
| 796 | 22 | 0.887 | 0.572 |
| 797 | 19 | 0.941 | 0.691 |
| 807 | 30 | 0.998 | 0.963 |
| 808 809 | 18 18 | 0.977 0.977 | 0.915 0.915 |
| 811 | 27 | 0.977 | 0.827 |
| 812 | 16 | 0.939 | 0.734 |
| 812 | 19 | 0.923 | 0.564 |
| 816 | 21 | 0.960 | 0.858 |
| 818 | 27 | 0.949 | 0.644 |
| 821 | 27 | 0.943 | 0.758 |
| 823 | 27 | 0.908 | 0.728 |
| 833 | 27 | 0.908 | 0.728 |
| 837 | 19 | 0.947 | 0.901 |
| 841 | 22 | 0.967 | 0.826 |
| 845 | 15 | 0.936 | 0.628 |
| 846 | 20 | 0.975 | 0.840 |
| 851 | 31 | 0.985 | 0.908 |
| 852 | 19 | 0.965 | 0.922 |
| 853 | 39 | 0.984 | 0.743 |
| 857 | 17 | 0.956 | 0.893 |
| 858 | 21 | 0.957 | 0.868 |
| 861 | 22 | 0.975 | 0.866 |
| <u> </u> | ٠ | | |

| 868 | 21 | 0.942 | 0.736 |
|-----|----|-------|-------|
| 871 | 43 | 0.973 | 0.560 |
| 873 | 19 | 0.952 | 0.730 |
| 874 | 33 | 0.923 | 0.717 |
| 879 | 23 | 0.978 | 0.911 |
| 881 | 16 | 0.947 | 0.884 |
| 887 | 17 | 0.970 | 0.916 |

TABLE 8

| SEQ ID NO: of Nucleotide Sequence | SEQ ID NO: of Polypeptide Sequence | SEQ ID NO: in USSN 09/659,671 |
|--------------------------------------|---------------------------------------|----------------------------------|
| 1 | 445 | 2 |
| 2 | 446 | 5 |
| 3 | 447 | 6 |
| 4 | 448 | 7 |
| 5 | 449 | |
| 6 | 450 | 9 |
| 7 | 451 | 11 |
| 8 | 452 | 12 |
| 9 | 453 | 13 |
| 10 | 454 | 14 |
| 11 | 455 | |
| 12 | | 15 |
| | 456 | 16 |
| 13 | 457 | 17 |
| 14 | 458 | 18 |
| 15 | 459 | 19 |
| 16 | 460 | 20 |
| 17 | 461 | 21 |
| 18 | 462 | 23 |
| 19 | 463 | 24 |
| 20 | 464 | 25 |
| 21 | 465 | 28 |
| 22 | 466 | 29 |
| 23 | 467 | 30 |
| 24 | 468 | 31 |
| 25 | 469 | 34 |
| 26 | 470 | 35 |
| 27 | 471 | 37 |
| 28 | 472 | 38 |
| 29 | 473 | 39 |
| 30 | 474 | 40 |
| 31 | 475 | 41 |
| 32 | 476 | 42 |
| 33 | 477 | 43 |
| 34 | 478 | 44 |
| 35 | 479 | 45 |
| 36 | 480 | 46 |
| 37 | 481 | 47 |
| 38 | 482 | 49 |
| 39 | 483 | 50 |
| 40 | 484 | 51 |
| 41 | 485 | 52 |
| 42 | 486 | 53 |
| 43 | 487 | 54 |
| 44 | 487 | 55 |
| 45 | | |
| | 489 | 56 |
| 46 | 490 | 57 |
| 47 | 491 | 58 |
| 48 | 492 | 59 |
| 49 | 493 | 60 |
| 50 | 494 | 61 |
| 51 | 495 | 62 |
| 52 | 496 | 63 |
| 53 | 497 | 64 |
| 54 | 498 | 65 |

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|------------|------------|------------|
| 55 | 499 | 66 |
| . 56 | 500 | 67 |
| 57 | 501 | 68 |
| 58 | 502 | 69 |
| 59 | 503 | 70 |
| 60 | 504 | 71 |
| 61 | 505 | 72 |
| 62 | 506 | 73 |
| 63 | 507 | 74 |
| 64 | 508 | 75 |
| 65 | 509 | 76 . |
| 66 | 510 | 77 |
| 67 | 511 | 78 |
| 68 | 512 | 79 |
| 69 | 513 | 80 |
| 70 | 514 | 81 |
| 71 | 515 | 82 |
| 72 | 516 | 83 |
| 73 | 517 | 85 |
| 74 | 518 | 86 |
| 75 | 519 | . 88 |
| 76 | 520 | 89 |
| 77 | 521 | 90 |
| 78 | 522 | 91 |
| 79 | 523 | 92 |
| 80 | 524 | 93 |
| 81 | 525 | 94 |
| 82 | 526 | 95 |
| 83 | 527 | 96 |
| 84 | 528 | 97 |
| 85 | 529 | 98 |
| 86 | 530 | 99 |
| 87 | 531 | 100 |
| 88 | 532 | 101 |
| 89 | 533 | 102 |
| 90 | 534 | 105 |
| 91 | 535 | 106 |
| 92 | 536 | 107 |
| 93 | 537 | 108 |
| 94 | 538 | 109 |
| 95 | 539 | 110 |
| 96 | 540 | 111 |
| 97 | 541 | 112 |
| 98 | 542 | 113 |
| 99 | 543 | 114 |
| 100 | 544 | 115 |
| 101 | 545 | 116 |
| 102 | 546 547 | 117 |
| 103 104 | 547 | 118 119 |
| 104 | 549 | 120 |
| 105 | 550 | 120 |
| 106 | 551 | 122 |
| 107 | 552 | 123 |
| 108 | 553 | 124 |
| 110 | 554 | 125 |
| 111 | 555 | 126 |
| 112 | 556 | 127 |
| 113 | 557 | 127 |
| | 558 | |
| 114 | 338 | 129 |

| | | • |
|------|-----|-----|
| 115 | 559 | 130 |
| 116 | 560 | 131 |
| 117 | 561 | 132 |
| 118 | 562 | 133 |
| 119 | 563 | 134 |
| 120 | 564 | 135 |
| 121 | 565 | 136 |
| 122 | 566 | 137 |
| 123 | 567 | 138 |
| 124 | 568 | 139 |
| 125 | 569 | 140 |
| 126 | 570 | 141 |
| 127 | 571 | 142 |
| 128 | 572 | 143 |
| 129 | 573 | 144 |
| 130 | 574 | 145 |
| 131 | 575 | 146 |
| 132 | 576 | 147 |
| 133 | 577 | 149 |
| 134 | 578 | 150 |
| 135 | 579 | 151 |
| 136 | 580 | 152 |
| 137 | 581 | 153 |
| 138 | 582 | 154 |
| 139 | 583 | 155 |
| 140 | 584 | 156 |
| 141 | 585 | 157 |
| 142 | 586 | 158 |
| 143 | 587 | 159 |
| 144 | 588 | 160 |
| 145 | 589 | 161 |
| 146 | 590 | 162 |
| 147 | 591 | 163 |
| 148 | 592 | 165 |
| 149 | 593 | 166 |
| 150 | 594 | 167 |
| 151 | 595 | 168 |
| 152 | 596 | 169 |
| 153 | 597 | 170 |
| 154 | 598 | 171 |
| 155 | 599 | 172 |
| 156 | 600 | 173 |
| 157 | 601 | 174 |
| 158 | 602 | 175 |
| 159 | 603 | 176 |
| 160 | 604 | 177 |
| 161 | 605 | 178 |
| 162 | 606 | 179 |
| 163. | 607 | 180 |
| 164 | 608 | 181 |
| 165 | 609 | 182 |
| 166 | 610 | 183 |
| 167 | 611 | 184 |
| 168 | 612 | 185 |
| 169 | 613 | 186 |
| 170 | 614 | 187 |
| 171 | 615 | 188 |
| 172 | 616 | 189 |
| 173 | 617 | 190 |
| 174 | 618 | 191 |
| | | |

| 175 | 619 | 192 |
|------------|------------|------------|
| 176 | 620 | 193 |
| 177 | 621 | 194 |
| 178 | 622 | 195 |
| 179 | 623 | 197 |
| 180 181 | 624 625 | 198 |
| 182 | 626 | 200 |
| 183 | 626 | 200 |
| 184 | 628 | 201 |
| 185 | 628 | 202 |
| 186 | 630 | 203 |
| 187 | 631 | 205 |
| 188 | 632 | 206 |
| 189 | 633 | 207 |
| 190 | 634 | 208 |
| 191 | 635 | 209 |
| 192 | 636 | 210 |
| 193 | 637 | 211 |
| 194 | 638 | 212 |
| 195 | 639 | 213 |
| 196 | 640 | 214 |
| 197 | 641 | 215 |
| 198 | 642 | 216 |
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WHAT IS CLAIMED IS:

- An isolated polynucleotide comprising a nucleotide sequence selected from the group consisting of SEQ ID NO: 1-444, a mature protein coding portion of SEQ ID NO: 1-444, an active domain coding portion of SEQ ID NO: 1-444, and complementary sequences thereof.
- An isolated polynucleotide encoding a polypeptide with biological activity, wherein said
 polynucleotide hybridizes to the polynucleotide of claim 1 under stringent hybridization
 conditions.
- An isolated polynucleotide encoding a polypeptide with biological activity, wherein said
 polynucleotide has greater than about 90% sequence identity with the polynucleotide of claim 1.
- 4. The polynucleotide of claim 1 wherein said polynucleotide is DNA.
- An isolated polynucleotide of claim 1 wherein said polynucleotide comprises the complementary sequences.
- 6. A vector comprising the polynucleotide of claim 1.
- 7. An expression vector comprising the polynucleotide of claim 1.
- 8. A host cell genetically engineered to comprise the polynucleotide of claim 1.
- A host cell genetically engineered to comprise the polynucleotide of claim 1 operatively
 associated with a regulatory sequence that modulates expression of the polynucleotide in the host
 cell.
- An isolated polypeptide, wherein the polypeptide is selected from the group consisting of:
 - a polypeptide encoded by any one of the polynucleotides of claim 1;
 and
 - a polypeptide encoded by a polynucleotide hybridizing under stringent conditions with any one of SEQ ID NO: 1-444.

- 11. A composition comprising the polypeptide of claim 10 and a carrier.
- 12. An antibody directed against the polypeptide of claim 10.
- 13. A method for detecting the polynucleotide of claim 1 in a sample, comprising:
- a) contacting the sample with a compound that binds to and forms a complex with the polynucleotide of claim 1 for a period sufficient to form the complex; and
- b) detecting the complex, so that if a complex is detected, the polynucleotide of claim 1 is detected.
- 14. A method for detecting the polynucleotide of claim 1 in a sample, comprising:
- a) contacting the sample under stringent hybridization conditions with nucleic acid primers that anneal to the polynucleotide of claim 1 under such conditions;
- b) amplifying a product comprising at least a portion of the polynucleotide of claim 1; and
- detecting said product and thereby the polynucleotide of claim 1 in the sample.
- 15. The method of claim 14, wherein the polynucleotide is an RNA molecule and the method further comprises reverse transcribing an annealed RNA molecule into a cDNA polynucleotide.
- 16. A method for detecting the polypeptide of claim 10 in a sample, comprising:
- a) contacting the sample with a compound that binds to and forms a complex with the polypeptide under conditions and for a period sufficient to form the complex; and
- detecting formation of the complex, so that if a complex formation is detected, the polypeptide of claim 10 is detected.
- 17. A method for identifying a compound that binds to the polypeptide of claim 10, comprising:
- a) contacting the compound with the polypeptide of claim 10 under conditions sufficient to form a polypeptide/compound complex; and
- b) detecting the complex, so that if the polypeptide/compound complex is detected, a compound that binds to the polypeptide of claim 10 is identified.

- 18. A method for identifying a compound that binds to the polypeptide of claim 10, comprising:
- a) contacting the compound with the polypeptide of claim 10, in a cell, under conditions sufficient to form a polypeptide/compound complex, wherein the complex drives expression of a reporter gene sequence in the cell; and
- b) detecting the complex by detecting reporter gene sequence expression, so that if the polypeptide/compound complex is detected, a compound that binds to the polypeptide of claim 10 is identified.
- 19. A method of producing the polypeptide of claim 10, comprising,
- a) culturing a host cell comprising a polynucleotide sequence selected from SEQ ID NO: 1-444, a mature protein coding portion of SEQ ID NO: 1-444, an active domain coding portion of SEQ ID NO: 1-444, complementary sequences thereof and a polynucleotide sequence hybridizing under stringent conditions to SEQ ID NO: 1-444, under conditions sufficient to express the polypeptide in said cell; and
 - b) isolating the polypeptide from the cell culture or cells of step (a).
- 20. An isolated polypeptide comprising an amino acid sequence selected from the group consisting of any one of the polypeptides SEQ ID NO: 217-432, or 649-864, the mature protein portion thereof, or the active domain thereof.
- 21. The polypeptide of claim 20 wherein the polypeptide is provided on a polypeptide array.
- 22. A collection of polynucleotides, wherein the collection comprising the sequence information of at least one of SEO ID NO: 1-444.
- 23. The collection of claim 22, wherein the collection is provided on a nucleic acid array.
- 24. The collection of claim 23, wherein the array detects full-matches to any one of the polynucleotides in the collection.
- 25. The collection of claim 23, wherein the array detects mismatches to any one of the polynucleotides in the collection.

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- 26. The collection of claim 22, wherein the collection is provided in a computer-readable format.
- 27. A method of treatment comprising administering to a mammalian subject in need thereof a therapeutic amount of a composition comprising a polypeptide of claim 10 or 20 and a pharmaceutically acceptable carrier.
- 28. A method of treatment comprising administering to a mammalian subject in need thereof a therapeutic amount of a composition comprising an antibody that specifically binds to a polypeptide of claim 10 or 20 and a pharmaceutically acceptable carrier.